AD NUMBER

AD374171

NEW LIMITATION CHANGE

TO

Approved for public release, distribution unlimited

FROM

Distribution authorized to U.S. Gov't. agencies and their contractors; Administrative/Operational Use; 10 JUN 1966. Other requests shall be referred to x.

AUTHORITY

.

AD NUMBER

AD374171

CLASSIFICATION CHANGES

TO

unclassified

FROM

confidential

AUTHORITY

30 Jun 1978, Gp-4 & OCA.

GENERAL DECLASSIFICATION SCHEDULE

IN ACCORDANCE WITH
DOD 5200.1-R & EXECUTIVE ORDER 11652

SECURITY MARKING

The classified or limited status of this report applies to each page, unless otherwise marked.
Separate page printouts MUST be marked accordingly.

THIS DOCUMENT CONTAINS INFORMATION AFFECTING THE NATIONAL DEFENSE OF THE UNITED STATES WITHIN THE MEANING OF THE ESPIONAGE LAWS, TITLE 18, U.S.C., SECTIONS 793 AND 794. THE TRANSMISSION OR THE REVELATION OF ITS CONTENTS IN ANY MANNER TO AN UNAUTHORIZED PERSON IS PROHIBITED BY LAW.

NOTICE: When government or other drawings, specifications or other data are used for any purpose other than in connection with a definitely related government procurement operation, the U. S. Government thereby incurs no responsibility, nor any obligation whatsoever; and the fact that the Government may have formulated, furnished, or in any way supplied the said drawings, specifications, or other data is not to be regarded by implication or otherwise as in any manner licensing the holder or any other person or corporation, or conveying any rights or permission to manufacture, use or sell any patented invention that may in any way be related thereto.

CONFIDENTIAL

NOLTR 65-217

COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U)

10 JUNE 1966

NOL

UNITED STATES NAVAL ORDNANCE LABORATORY, WHITE OAK, MARYLAND

NOLTR 65-217

CONFIDENTIAL

COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U)

By
Harold Hurwitz

ABSTRACT: The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY. In general, the calculated detonation properties of the fluorinated explosives, compared with the properties of the non-fluorinated parent compounds, showed increased detonation velocity, increased detonation pressure, and decreased detonation energy. It should be noted that if lower densities had been assumed, the computed detonation pressures and velocities would have been lower. For example, the computed detonation velocity for 2,2,4,6-tetrafluoro-RDX at the initial density ρ_0 = 2.17 gm/cc is 9.25 mm/μsec (compared with 8.80 for RDX at TMD), and the computed detonation pressure is 0.409 megabars (compared with 0.344 for RDX). At ρ_0 = 2.05 gm/cc, the values computed for the same compound are 8.65 mm/μsec and 0.352 megabars. Computed detonation velocities of the fluorinated TNB's at measured densities show an average deviation of 2.1% from literature values.

EXPLOSION DYNAMICS DIVISION
EXPLOSIONS RESEARCH DEPARTMENT
U. S. NAVAL ORDNANCE LABORATORY
WHITE OAK, MARYLAND

NOLTR 65-217 10 June 1966

COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U)

The work described in this report was carried out under Eglin Air Force Base MIPR PG-3-19, dated September 1963. The purpose of the work was to calculate the detonation properties of a number of fluoroexplosives. This makes possible a preliminary evaluation of the compounds, thus serving as a guide for possible experimental effort.

J. A. DARE
Captain, USN
Commander

D. Kabek, for

C. J. ARONSON
By directon

TABLE OF CONTENTS

TABLES

ILLUSTRATIONS

ILLUSTRATIONS CONTINUED

COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U)

INTRODUCTION

1. The research described in this report was conducted by the Naval Ordnance Laboratory for the Air Force under Eglin Air Force Base MIPR PG-3-19, dated September 1963. Under this contract NOL was to calculate the detonation properties of a number of fluorinated explosive compounds. Previously, the Denver Research Institute on an Air Force contract had shown by chemical synthesis and subsequent measurements that the replacement of hydrogen atoms by fluorine atoms in explosive materials could lead to improvements in desirable properties (Ref. 1).* The need for actual synthesis and measurement, however, could be kept to a minimum by the use of available computational methods that predict the properties of hypothetical compounds.

2. Detonation characteristics of explosive compositions can be estimated using the RUBY code, a digital computer program developed at the Lawrence Radiation Laboratories (Ref. 2) and now in use at NOL (Refs. 3,4). An important feature of RUBY is the use of the Kistiakowsky-Wilson equation of state (which may be written as in Equation (1)) to represent the behavior of the explosion product gases.

$$PV/RT = 1 + x \exp(\beta x)$$

$$x = k/V(T + \theta)^{\alpha} \qquad (1)$$

$$k = \kappa \sum_i x_i k_i$$

In Equation (1), V is the molar gas volume, P is the pressure, T is the absolute temperature, and x_i is the mole fraction of component i. The quantities α, β, κ, θ, and k_i are constants, the k_i being covolumes. The use of this equation of state for representing gaseous explosion products has been discussed by Mader (Ref. 5).

3. Certain properties of the explosive material (HE) and the product species are required as input to RUBY. For the HE these are chemical composition, density, and heat of formation. The input quantities required for the gaseous product species are chemical composition, thermodynamic properties, and covolumes (k_i). The only condensed product considered in the present work is solid graphite, and the information on graphite required as input to RUBY includes thermodynamic properties, molar volume, and constants for an appropriate equation of state (note that Equation (1) applies only to gases). The equation of state used for this purpose is

$$P = -2.4673 + 6.7692Y - 6.9555Y^2 + 3.0405Y^3 - 0.3869Y^4$$
$$+(-1.9534 + 2.3368Y) \times 10^{-5}T$$
$$+(6.1742 - 5.794/Y + 2.277/Y^2) \times 10^{-10}T^2$$
$$Y = \frac{V_o}{V},$$

*References may be found on page 8.

where P is in megabars, and T in degrees Kelvin, as given in Refs. 2 and 6.

4. In this report, lengthy chemical names have been abbreviated to short symbols for convenience. These short names are defined in Table 1, which also includes definitions of conventional HE names (RDX, DATB, etc.). The explosives investigated were mono-, di-, and trifluorinated TNB; mono-, di-, and tetrafluorinated RDX; mono- and difluorinated tetryl; mono- and difluorinated TNT; fluorinated DATB; trinitrobenzotrifluoride, and its mono- and difluoro derivatives; and fluorodinitropropane, fluorodinitromethane, and mixtures of the two. In general, the calculated detonation properties, compared with the properties of the non-fluorinated parent explosive compounds, show increased detonation velocity and detonation pressure, and decreased detonation energy.

SOURCES OF INPUT DATA

5. The thermodynamic properties--enthalpy of formation, Gibbs free energy of formation, and constants giving the constant-pressure heat capacity as a function of temperature--required for the product species, were obtained from the JANAF Thermochemical Tables (Ref. 7). Covolumes used for the gaseous products were those given in Ref. 8, with the revisions for H_2O and CO_2 suggested in Ref. 5.

6. The heats of formation (ΔH_f) required for hypothetical explosive compositions had to be estimated. There are a number of useful methods (e.g. Refs. 9 and 10) for estimating heats of formation by summing the contributions of various structural features over the entire molecule. However, since the compounds treated in the present work are simple derivatives of known chemical species, the estimation of their heats of formation was approached by taking as a starting point molecules whose heats of formation were already known. The method may be illustrated by taking monofluorodiaminotrinitrobenzene (FDATB) as an example:

$$C_6H_6(\ell) \xrightarrow{F} C_6H_5F(\ell)$$

ΔH_f = +11.7 kcal/mole ΔH_f = -34.8

$$\Delta H = -34.8-11.7 = -46.5$$

$$\text{DATB (s)} \xrightarrow{F} \text{FDATB (s)}$$

ΔH_f = -29.2 ΔH_f = ?

$$\Delta H_f(\text{FDATB}) = -29.2 + (-46.5) = -75.7 \text{ kcal/mole}$$

The difference in heat of formation between benzene and monofluorobenzene is -46.5 kcal/mole. When this is added to the heat of formation of DATB (-29.2 kcal/mole) the result is -75.7 kcal/mole, the estimated heat of formation of FDATB. In this procedure, the ΔH_f difference due to

fluorination of a liquid to form a liquid is assumed to be approximately equal to the ΔH_f difference due to fluorination of a solid to form another solid. Appendix A shows the computation of the ΔH_f estimates for the various compounds treated in this report. The resulting estimated ΔH_f values are listed in Table 2.

7. In making the detonation calculations for the hypothetical compositions it is also necessary to estimate densities. Pavlath and Leffler (Ref. 11) suggest that densities be estimated by examining the molar volumes of similar compounds rather than from densities of similar compounds directly. Although these authors stress that their method is strictly applicable only to liquids, in the present work it was considered to give an adequate approximation for solids when no other information was available. It should be noted that the computed detonation properties are strongly influenced by these density estimates. Consideration of other factors which sometimes affect the densities of solids (such as charge distribution and symmetry) might have led to lower densities and lower detonation velocities and pressures.

8. Table 3 gives the densities used for the RUBY calculations. In the case of the fluorinated trinitrobenzenes, only one density for each compound is given in the table although RUBY computations were also carried out for other densities for comparison with results reported by other investigators. Two separate densities are listed as estimated for each fluorinated RDX, and computations were carried out for each value. This was done because the volume increment derived by Pavlath and Leffler for aromatic compounds could not be applied with confidence to the aliphatic RDX's. For the TNBTF's the method of applying the theory to the side-chain fluorine atoms was uncertain, and the estimates are consequently given to only two significant figures.

9. The values of the equation-of-state parameters α, β, κ, and θ are those given by Mader in Ref. 5. The values of k_i were those given in Ref. 8 with the changes suggested in Ref. 5. The quantities α and β are dimensionless, the k_i have the dimensions of volume, θ has the dimensions of temperature, and κ has the dimensions of temperature raised to the α power. For β and κ, Mader recommended two sets of values. One set (called here RDX-type) is fitted to the properties of RDX, but then adjusted so that $(\partial P/\partial T)_v$ will always be positive. The other set (called here TNT-type) is fitted to the properties of TNT and recommended for dense explosives whose products contain relatively large amounts of solid graphite. The values of α, β, κ, and θ are as follows:

$\alpha = 0.50$

$\theta = 400°K$

Parameter Type	β	$\mathring{A}$ ($°K^{\alpha}$)
TNT	0.0958	12.685
RDX	0.16	10.91

The values of the k_i are given in Table 4. It should be noted that consistency with the use of cubic centimeters as the units for other volume quantities in the computation requires that the units of the k_i be considered as cubic centimeters. However, as is usual in RUBY-type computations, the numerical values of Mader's k_i, which are computed in terms of cubic angstroms per molecule, have been used here without application of the appropriate factor (0.602) to convert to cubic centimeters per mole. This is equivalent to multiplying each k_i by 1.66, which is the reciprocal of the conversion factor.

RESULTS OF COMPUTATIONS

10. Because of the uncertainty in some of the heat of formation estimates, it was of interest to observe the effect of changes in the heat of formation of the explosive composition on RUBY results. For this purpose, and also to compare the effects of the two sets of values of β and κ, computations were carried out for MFTNT assuming the ΔH_f to be -50, -75, and -100 kcal/mole and using both sets of the equation of state parameters. The results are shown in Table 5, and in Figures 1, 2, and 3. In Tables 5-11, P, T, ρ, E, and S are pressure, temperature, density, energy, and entropy, respectively. The subscript J indicates the detonation products in the Chapman-Jouguet state, and the subscript o indicates the unreacted explosive at 298°K and 1 atm. pressure. ΔE_{chem} is the detonation energy, defined as the energy increase while going from the unreacted explosive at 298°K and 1 atm. pressure, to the Chapman-Jouguet gas mixture reduced to 298°K and 1 atm. pressure.

11. Decreasing the ΔH_f of the MFTNT from -50 to -100 kcal/mole, using the TNT-type parameters, caused a 3.0% decrease in the computed detonation velocity, an 8.1% decrease in the Chapman-Jouquet (CJ) pressure, and a 451°K (or 16.0%) drop in the CJ temperature. The energy change for the chemical reaction (ΔE_{chem}) increased by 200 cal/gm or 49.0 kcal/mole, a value which suggests an immediate derivation from the decrease in ΔH_f of the explosive. The change in composition of the product mixture can be considered to result from a shift to the right of the equilibrium reaction

$$4HF + 8CO \rightleftharpoons CF_4 + 3CO_2 + 4C + 2H_2O \ . \qquad (2)$$

Such a shift would be expected to be associated with the decrease in temperature, although it would be opposed by the decrease in pressure.

12. When the computations using the two sets of equation-of-state parameters are compared (both for ΔH_f = -50 kcal/mole), it is seen that with the RDX-type parameters the detonation velocity is 5.2% higher, the CJ pressure is 5.2% higher, and the CJ temperature is 6.2% lower. The difference in ΔE_{chem} is negligible (0.16%). The difference in chemical composition of the product mixture can again be described as a righthand shift in Equation 2 (for a change from TNT-type parameters to RDX-type parameters), with the increase in pressure and decrease in temperature now acting in the same direction.

13. RUBY computations were carried out for a series of fluorinated RDX's. The results are given in Table 6 for 0,1,2, and 4 fluorine atoms per molecule. The program would not converge for the trifluoro-RDX's. The detonation velocities, CJ pressures, and chemical energies are plotted in Figures 4, 5, and 6, respectively, the points for the difluoro and tetrafluoro compounds being plotted for the more probable higher densities (see paragraph 8).

14. It can be seen from the graphs that as the number of fluorine atoms per molecule increases, the detonation velocity increases, the CJ pressure increases, and the detonation energy ($-\Delta E_{chem}$) decreases. Although the ΔE_{chem} (Figure 6) seems to be strictly monotonic, the D and P_J curves (Figures 4 and 5) have humps at the two-fluorine-atom position. However, the estimated density of the difluoro-RDX is likely a few tenths of a percent too high, and a correction of this magnitude would smooth out the D and P_J curves. For the disubstituted and tetrasubstituted compounds, the differences between isomers are presented to RUBY simply as differences in heat of formation. Accordingly, the consequent differences in computed results are analogous to those discussed in paragraph 11.

15. Computed detonation parameters for fluorinated TNB, tetryl, TNT, TNBTF, and DATB are given in Tables 7-10, along with values computed for the unfluorinated materials for comparison. (See Figures 7-9 for plots of TNB results.) Since it was not clear which set of equation-of-state parameters was applicable in each case, computations were carried out using both sets, and both are listed in the tables.

16. Table 11 gives the results of computations suggested by Dr. J. M. Rosen of this Laboratory, for FDNP, FTNM, and mixtures of the two. As predicted by Rosen (Ref. 12) the maximum detonation energy is computed for a mixture containing approximately 50.3% FDNP, which is balanced for complete reaction to H_2O, CO_2, CF_2, and N_2. The P_J maximum is at about the same composition, while the mixture with maximum detonation velocity seems to contain a little more FDNP.

COMPARISON WITH OTHER VALUES

17. Experimentally determined detonation velocities for several of the compounds treated here have been reported by other workers (Refs. 1, 13, 14). These values are given in Table 12, along with values computed by Amcel using RUBY (Ref. 14), and NOL RUBY results. The same information is presented graphically for DFTNB, MFTNB, and TNBTF in Figures 10, 11, and 12.

18. For MFTNB, DFTNB, and TFTNB, computations were carried out at the same loading densities (ρ_o) at which experimental detonation velocities had been reported by Schmidt-Collerus et al of the Denver Research Institute (Ref. 1). The RDX parameters were used for this comparison because, as seen in the Table, they seemed to give results that were closer to the experimental values.

19. For MFTNB at ρ_o = 1.512, 1.615, and 1.802 gm/cc, the deviations of the NOL computed values from the DRI experimental values are +0.14%, -1.6%, and +0.17%. Deviation from the Picatinny value (Ref. 13) at ρ_o = 1.80 is +4.8%. If the value computed at NOL for ρ_o = 1.8383 (RDX parameters) is compared with the experimental value reported by Amcel for ρ_o = 1.83, the deviation is +0.026%.

20. For DFTNB the deviations from the DRI experimental values are not quite as good. For ρ_o = 1.695, 1.768, and 1.841, the deviations are -3.7%, -3.5%, and -3.0%, respectively. The deviation from the Picatinny value at ρ_o = 1.84 is -0.94%. The deviation of the NOL computed value at ρ_o = 1.8564 (RDX parameters) from the Amcel experimental value at ρ_o = 1.855 is -2.1%. It should be noted that the NOL-estimated heat of formation of DFTNB is 100% greater than that found by Amcel. If the Amcel value is correct, this would account for the relatively large deviations for this compound, recalling that for MFTNT a similar difference in the heat of formation used for input produced a 2.1% decrease in the computed value of D (using RDX parameters).

21. For TFTNB at ρ_o = 1.964, the deviation from the DRI experimental value is +1.3%. Literature values for TNBTF, MFTNBTF, and DFTNBTF are listed in the Table, but NOL computations were not carried out at densities appropriate for comparison.

22. In the Amcel computations (results listed in Table 12) the older values of the equation of state parameters were used, and the carbon formed in the reaction was assumed incompressible. The resulting computed detonation properties may be useful for intercomparison of certain compounds, whether or not they are considered valid predictions of absolute values. Since the Amcel and NOL RUBY computations are based on different assumptions, the results necessarily disagree.

CONCLUSIONS

23. According to the computed results presented in this report, fluorination of C-H-N-O explosives promises improved performance in applications where relatively high detonation velocities and pressures are desirable but high energy is not required. (This is not consistent with the high energy outputs referred to in Ref. 1.) The RUBY computations for progressively fluorinated RDX, TNT, and DATB all show an increase in detonation velocity and Chapman-Jouguet pressure as the number of F atoms in the molecule is increased, with an accompanying decrease in the detonation energy (assuming each compound is at crystal density). For tetryl and TNBTF, the computations show an increase in P_J and D when RDX-type parameters are used, although when TNT-type parameters are used the computed values of these properties decrease on addition of the first F atom, with subsequent increase on additional fluorination. This suggests that the RDX-type parameters give the more valid results for these two series of compounds. The computations for the fluorinated TNB's show an irregular effect on P_J and D of progressive fluorination, but this may actually result from the difficulty of estimating heats of formation and densities. The computed $-\Delta E_{chem}$ for the fluorinated TNB's shows the usual steady decrease.

24. The contract under which the present work was carried out (see paragraph 1) suggests that the most promising materials might be those with a stoichiometric balance to HF. If the results for the fluorinated RDX's (Figures 4-6) are examined from this standpoint, an apparent change in slope can be observed near the HF balance point (3 fluorine atoms in the molecule). This feature of the RDX curves, however, can be explained with equal validity as being related to the HF balance or as resulting from errors in the estimates of densities and heats of formation. The ranges of fluorination of the other series of compounds treated did not include the HF balance point.

REFERENCES

1. Josef J. Schmidt-Collerus, John A. Young, John A. Drimmel, et al, (Denver Research Institute), Research on Fluoroexplosives Report ATL-TDR-64-45 Contract No. AF 08(635)-2109. Directorate of Armament Development, Det 4, Research and Technology Division, Air Force Systems Command, Eglin Air Force Base, Florida, July 1964.

2. Howard B. Levine and Robert E. Sharples, Operator's Manual for RUBY. Report UCRL 6815, University of California, Ernest O. Lawrence Radiation Laboratory, Livermore, California, March 20, 1962.

3. H. Hurwitz, Calculation of Detonation Parameters with the RUBY Code, NOLTR 63-205. U. S. Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland, March 31, 1965.

4. Donna Price and Harold Hurwitz, RUBY Code Calculation of Detonation Properties I. C-H-N-O Systems, NOLTR 63-216. U. S. Naval Ordnance Laboratory, Silver Spring, Maryland, November 1, 1963.

5. Charles L. Mader, Detonation Properties of Condensed Explosive Computed Using the Becker-Kistiakowsky-Wilson Equation of State. Report LA-2900. Los Alamos Scientific Laboratory of the University of California, Los Alamos, New Mexico. Written February 19, 1963. Distributed July 17, 1963.

6. R. D. Cowan and W. Fickett, Calculation of the Detonation Properties of Solid Explosives with the Kistiakowsky-Wilson Equation of State. J. Chem. Phys. 24, 932 (1956).

7. JANAF Thermochemical Tables, as Supplemented, 1962. (Walter H. Jones, Chairman, JANAF Thermochemical Panel) Dow Chemical Company, Midland, Mich.

8. Charles L. Mader, Detonation Performance Calculations Using the Kistiakowsky-Wilson Equation of State. Report LA-2613. Los Alamos Scientific Laboratory of the University of California, Los Alamos, New Mexico. Written January 1961. Distributed October 9, 1961.

9. Keith J. Laidler, A System of Molecular Thermochemistry for Organic Gases and Liquids. Can. J. Chem. 34, 626-48 (1956).

10. G. Richard Handrick, Heats of Combustion of Organic Compounds, I&E Chem. 48 1366 (1956).

11. Attila E. Pavlath and Amos J. Leffler, Aromatic Fluorine Compounds. ACS Monograph No. 155. (Reinhold Publ. Co., New York, 1962).

12. J. M. Rosen Private Communication, U. S. Naval Ordnance Laboratory, White Oak, Maryland.

REFERENCES

13. Picatinny Arsenal Monthly Progress Report No. 1, MIPR PG-3-20 1 November 1963. (Cited in Reference 1).

14. Fred M. Hudson and Staff (Amcel Propulsion Company), Evaluation of New Explosive Mixtures. Technical Report No. ATL-TDR-64-12, Contract No. AF 08 (635)-3650. Directorate of Armament Development, Det. 4, Research and Technology Division, Air Force Systems Command, Eglin Air Force Base, Florida, October 1964.

15. W. D. Good, D. W. Scott, and Guy Waddington, Combustion Calorimetry of Organic Fluorine Compounds by a Rotating Bomb Method. J. Phys. Chem. 60, 1080 (1956).

16. F. D. Rossini, et al, Selected Values of Properties of Hydrocarbons. Circular of the Natl. Bureau of Standards C-461. November 1947.

17. W. D. Good, et al, Combustion Calorimetry of Organic Fluorine Compounds. The Heats of Combustion and Formation of the Difluorobenzenes, 4-Fluorotoluene, and m-Trifluorotoluic Acid. J. Phys. Chem. 66, 1529 (1962).

18. W. D. Good, et al, Thermochemistry and Vapor Pressure of Aliphatic Fluorocarbons. A Comparison of the C-F and C-H Thermochemical Bond Energies. J. Phys. Chem. 63, 1133 (1959).

TABLE 1. DEFINITION OF NAMES USED FOR CHEMICAL COMPOUNDS

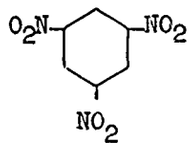
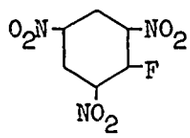
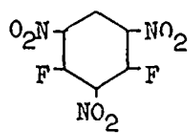
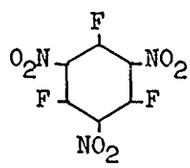
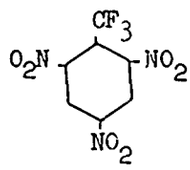
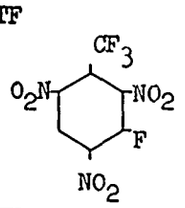
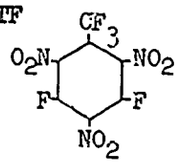
TNB		Trinitrobenzene $C_6H_3N_3O_6$ MW = 213.11
MFTNB		Monofluorotrinitrobenzene $C_6H_2N_3O_6F$ MW = 231.10
DFTNB		Difluorotrinitrobenzene $C_6HN_3O_6F_2$ MW = 249.09
TFTNB		Trifluorotrinitrobenzene $C_6N_3O_6F_3$ MW = 267.08
TNBTF		Trinitrobenzotrifluoride $C_7H_2N_3O_6F_3$ MW = 281.11
MFTNBTF		Monofluorotrinitrobenzotrifluoride $C_7HN_3O_6F_4$ MW = 299.10
DFTNBTF		Difluorotrinitrobenzotrifluoride $C_7N_3O_6F_5$ MW = 317.09

TABLE 1 Contd

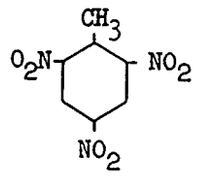
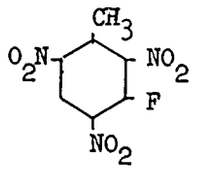
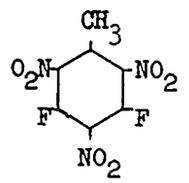
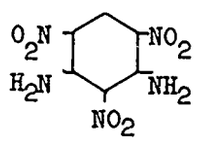
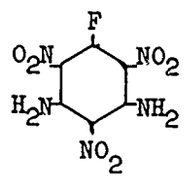
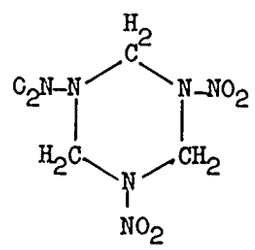
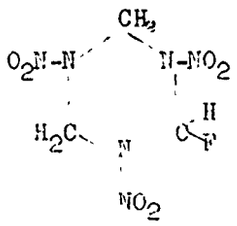
TNT		Trinitrotoluene $C_7H_5N_3O_6$ MW = 227.13
MFTNT		Monofluorotrinitrotoluene $C_7H_4N_3O_6F$ MW = 245.12
DFTNT		Difluorotrinitrotoluene $C_7H_3N_3O_6F_2$ MW = 263.12
DATB		Diaminotrinitrobenzene $C_6H_5N_5O_6$ MW = 243.14
FDATB		Fluorodiaminotrinitrobenzene $C_6H_4N_5O_6F$ MW = 261.13
RDX		1,3,5-Trinitrohexahydro-s-triazine (or Cyclotrimethylenetrinitramine) $C_3H_6N_6O_6$ MW = 222.12

Table 1 Contd

MFRDX

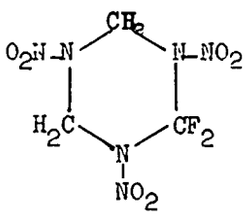


2-Fluoro-1,3,5-trinitrohexahydro-s-triazine

$C_3H_5N_6O_6F$

MW = 240.11

22DFRDX

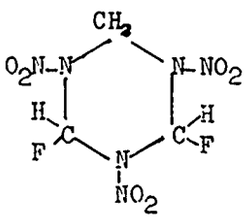


2,2-Difluoro-1,3,5-trinitrohexahydro-s-triazine

$C_3H_4N_6O_6F_2$

MW = 258.10

24DFRDX

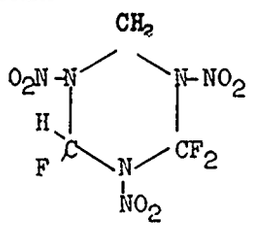


2,4-Difluoro-1,3,5-trinitrohexahydro-s-triazine

$C_3H_4N_6O_6F_2$

MW = 258.10

224TFRDX

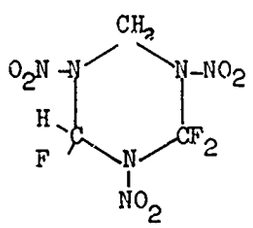


2,2,4-Trifluoro-1,3,5-trinitrohexahydro-s-triazine

$C_3H_3N_6O_6F_3$

MW = 276.09

246TFRDX

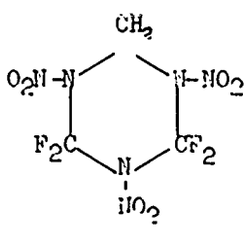


2,4,6-Trifluoro-1,3,5-trinitrohexahydro-s-triazine

$C_3H_3N_6O_6F_3$

MW = 276.09

2244TTFRDX



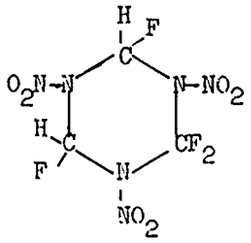
2,2,4,4-Tetrafluoro-1,3,5-trinitrohexahydro-s-triazine

$C_3H_2N_6O_6F_4$

MW = 294.08

Table 1 Contd

2246TTFRDX

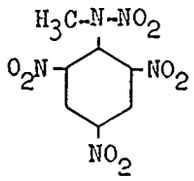


2,2,4,6-Tetrafluoro-1,3,5-trinitrohexahydro-s-triazine

$C_3H_2N_6O_6F_4$

MW = 294.08

Tetryl

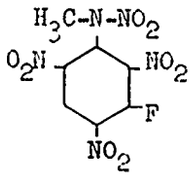


Trinitrophenylmethylnitramine

$C_7H_5N_5O_8$

MW = 287.15

MFT

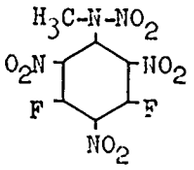


Monofluorotrinitrophenylmethylnitramine

$C_7H_4N_5O_8F$

MW = 305.14

DFT

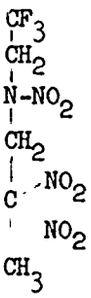


Difluorotrinitrophenylmethylnitramine

$C_7H_3N_5O_8F_2$

MW = 323.13

TFNA



1,1,1-Trifluoro-3,5,5-trinitro-3-azahexane

$C_5H_7N_4O_6F_3$

MW = 276.13

Table 1 Contd

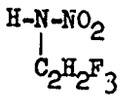
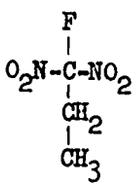
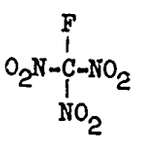
TFENA		Trifluoroethyl nitramine $C_2H_3N_2O_2F_3$ MW = 144.05
FDNP		Fluorodinitropropane $C_3H_5N_2O_4F$ MW = 152.05
FTNM		Fluorotrinitromethane CN_3O_6F MW = 169.03

TABLE 2. ESTIMATED HEATS OF FORMATION

HE	ΔH_f (Kcal/mole)	HE	ΔH_f (Kcal/mole)
MFTNB	-58	MFRDX	-26
DFTNB	-103	22DFRDX	-76
TFTNB	-148	24DFRDX	-66
TNBTF	-171	224TFRDX	-116
MFTNBTF	-216	246TFRDX	-106
DFTNBTF	-262	2244TTFRDX	-166
MFTNT	-64	2246TTFRDX	-156
DFTNT	-109	MFT	-42
FDATB	-76	DFT	-87

TABLE 3. DENSITIES OF EXPLOSIVE MATERIALS USED FOR RUBY CALCULATIONS

HE	ρ (gm/cc)	Reference
MFTNB	1.8383	1
DFTNB	1.8564	1
TFTNB	1.9477	1
TNBTF	1.9	Estimated
MFTNBTF	2.0	Estimated
DFTNBTF	2.1	Estimated
MFTNT	1.79	Estimated
DFTNT	1.88	Estimated
FDATB	1.97	Estimated
MFRDX	1.90,1.87	Estimated
22DFRDX	2.00,1.94	Estimated
24DFRDX	2.00,1.94	Estimated
224TFRDX	2.09,2.00	Estimated
246TFRDX	2.09,2.00	Estimated
2244TTFRDX	2.17,2.05	Estimated
2246TTFRDX	2.17,2.05	Estimated
MFT	1.84	Estimated
DFT	1.92	Estimated
TFNA	1.692	5
TFENA	1.523	5
FDNP	1.35	12
FTNM	1.586	12

TABLE 4 COVOLUMES (k_i) USED IN THE RUBY COMPUTATIONS

Species	k_i (cc/mole)	Species	k_i (cc/mole)	Species	k_i (cc/mole)
CF_2	1330	CO_2	600	N_2	380
CF_3	1330	COF_2	1300	N_2O	600
CF_4	1330	F	108	NH_3	476
CH_2F_2	1330	F_2	387	NO	386
CH_3F	1920	H	76	NO_2	600
CH_4	528	H_2	180	O	120
CHF_3	1920	H_2O	250	O_2	350
CO	390	HF	389	OH	413

TABLE 5. COMPUTED DETONATION PROPERTIES FOR MFTNT, USING DIFFERENT ΔH_f's AND EQUATION-OF-STATE PARAMETERS

Property		Units						
(Parameter Type)			TNT	TNT	TNT	RDX	RDX	RDX
ΔH_f		kcal/mole	-50	-75	-100	-50	-75	-100
ρ_o		gms/cc	1.80	1.80	1.80	1.80	1.80	1.80
D		mm/μsec	7.292	7.186	7.079	7.668	7.588	7.510
P_J		megb	0.2465	0.2366	0.2266	0.2592	0.2500	0.2410
T_J		°K	2818.	2593.	2367.	2643.	2413.	2182.
ρ_J		gms/cc	2.425	2.414	2.404	2.384	2.372	2.360
γ			2.882	2.930	2.981	3.083	3.146	3.212
E_J-E_o		cal/gm HE	421.7	399.7	377.8	421.5	400.4	379.9
ΔE_{chem}		cal/gm HE	-1265.	-1166.	-1065.	-1267.	-1167.	-1066.
S_J-S_o		cal/°K/gm/HE	0.05853	0.01639	-0.02947	0.06576	0.02199	-0.02596
Composition of Product Mixture	CF_2	10^{-3} moles/gm HE	*	*	*	*	*	*
	CF_3		*	*	*	*	*	*
	CF_4		0.9379	0.9544	0.9698	0.9651	0.9805	0.9936
	CH_2F_2		*	*	*	*	*	*
	CH_3F		*	*	*	*	*	*
	CH_4		*	*	*	*	*	*
	CHF_3		*	*	*	*	*	*
	CO		0.3960	0.2422	0.1340	0.2488	0.1434	0.0620
	CO_2		8.045	8.105	8.143	8.090	8.132	8.154
	COF_2		*	*	*	*	*	*
	F		*	*	*	*	*	*
	F_2		*	*	*	*	*	*
	H		*	*	*	*	*	*
	H_2		*	*	*	*	*	*
	H_2O		7.991	8.025	8.057	8.049	8.080	8.106
	HF		0.3272	0.2616	0.2004	0.2186	0.1574	0.1050
	N_2		6.118	6.118	6.119	6.119	6.119	6.119
	N_2O		*	*	*	*	*	*
	NH_3		*	*	*	*	*	*
	NO		*	*	*	*	*	*
	NO_2		*	*	*	*	*	*
	O		*	*	*	*	*	*
	O_2		*	*	*	*	*	*
	OH		*	*	*	*	*	*
C(graphite)			19.18	19.26	19.31	19.25	19.31	19.35
Σ moles gas		10^{-3} moles/gm HE	23.82	23.71	23.62	23.69	23.60	23.54
V_g		cc/mole	14.18	14.29	14.39	14.58	14.70	14.81
V_s		cc/mole	3.892	3.913	3.936	3.847	3.864	3.881

*Mole fraction in gas mixture less than 10^{-4}.

TABLE 6. COMPUTED DETONATION PROPERTIES FOR FLUORINATED RDX's
(Using RDX-Type Parameters)

Property		Units	RDX	MFRDX	22DFRDX	22DFRDX	24DFRDX	24DFRDX	2244TTFRDX	2244TTFRDX	2246TTFRDX	2246TTFRDX
ΔH_f		kcal/mole	+14.71	-26	-76	-76	-66	-66	-166	-166	-156	-156
ρ_o		gms/cc	1.802	1.90	2.00	1.94	2.00	1.94	2.17	2.05	2.17	2.05
D		mm/μsec	8.804	8.940	9.091	8.830	9.107	8.840	9.252	8.642	9.254	8.652
P_J		megb	0.3442	0.3676	0.3886	0.3505	0.3921	0.3641	0.4056	0.3487	0.4089	0.3518
T_J		°K	2568.	2335.	2005.	2147.	2095.	2240.	1241.	1493.	1311.	1572.
ρ_J		gms/cc	2.391	2.507	2.615	2.549	2.619	2.553	2.776	2.655	2.782	2.660
γ			3.058	3.131	3.254	3.186	3.231	3.163	3.579	3.391	3.544	3.362
E_J-E_o		cal/gm HE	562.4	559.6	545.9	530.6	553.8	538.7	487.8	463.0	495.6	470.1
ΔE_{chem}		cal/gm HE	-1500.	-1424.	-1322.	-1322.	-1360.	-1360.	-1018.	-1020.	-1052.	-1054.
S_J-S_o		cal °K gm HE	-0.2076	-0.2388	-0.2922	-0.2548	-0.2741	-0.2400	-0.4667	-0.3760	-0.4398	-0.3531
Composition of Product Mixture	CF_2	10^{-3}mole/gm HE	-	-	-	-	-	-	-	-		-
	CF_3		-	-	-	-	-	-	-	-	-	-
	CF_4		-	1.036	1.937	1.935	1.936	1.935	3.400	3.400	3.400	3.400
	CH_2F_2		-	-	-	-	-	-	-	-	-	-
	CH_3F		-	-	-	-	-	-	-	-	-	-
	CH_4		*	*	*	*	*	*	*	*	*	*
	CHF_3		-	-	-	-	-	-	-	-	-	-
	CO		0.1171	0.03237	0.004000	0.01190	0.006352	0.01771	*	*	*	*
	CO_2		6.694	7.277	7.748	7.745	7.747	7.743	6.801	6.801	6.801	6.801
	COF_2		-	-	-	-	-	-	-	-	-	-
	F		-	*	*	*	*	*	*	*	*	*
	F_2		-	*	*	*	*	*	*	*	*	*
	H		-	-	-	-	-	-	-	-	-	-
	H_2		-	*	*	*	*	*	*	*	*	*
	H_2O		13.51	10.40	7.748	7.745	7.747	7.743	3.400	3.400	3.400	3.400
	HF		-	0.01895	*	0.008152	0.003405	0.01088	*	*	*	*
	N_2		13.51	12.49	11.62	11.62	11.62	11.62	9.596	9.731	9.592	9.726
	N_2O		-	*	*	*	*	*	0.04965	0.04899	0.05910	0.05687
	NH_3		*	*	*	*	*	*	*	*	*	*
	NO		-	*	*	*	*	*	*	*	*	0.002859
	NO_2		-	*	*	*	*	*	1.112	0.8405	1.101	0.8330
	O		-	-	-	-	-	-	-	-	-	-
	O_2		-	*	*	*	*	*	0.5636	0.8343	0.5697	0.8373
	OH		-	-	-	-	-	-	-	-	-	-
	C(graphite)		6.694	4.149	1.935	1.931	1.934	1.928	0.0	0.0	0.0	0.0
Σ moles gas		10^{-3}moles/gm HE	33.82	31.26	29.06	29.07	29.06	29.07	24.92	25.06	24.92	25.06
V_g		cc/mole	11.65	12.29	12.92	13.26	12.90	13.23	14.45	15.03	14.42	15.00
V_s		cc/mole	3.635	3.579	3.529	3.587	3.526	3.583	3.477	3.589	3.473	3.586

*Mole fraction in gas mixture less than 10^{-4}

TABLE 7. COMPUTED DETONATION PROPERTIES FOR FLUORINATED TNB's

Property		Units	TNB	MFTNB	DFTNB	TFTNB	MFTNB	DFTNB	TFTNB
(Parameter Type)			RDX	RDX	RDX	RDX	TNT	TNT	TNT
ΔH_f		kcal/mole	-11.40	-58.	-103.	-148.	-58.	-103.	-148.
ρ_o		gms/cc	1.688	1.8383	1.8564	1.9477	1.8383	1.8564	1.9477
D		mm/μsec	7.371	7.657	7.459	7.541	7.242	7.009	6.982
P_J		megb	0.2299	0.2647	0.2525	0.2640	0.2500	0.2365	0.2418
T_J		°K	2990.	2703.	2625.	2423.	2914.	2862	2723.
ρ_J		gms/cc	2.253	2.437	2.457	2.557	2 482	2.506	2.613
γ			2.989	3.071	3.090	3.196	2.856	2.856	2.926
E_J-E_o		cal/gm HE	408.1	422.7	397.5	385.9	421.5	394.9	377.8
ΔE_{chem}		cal/gm HE	-1340.	-1261.	-1188.	-1125.	-1257.	-1184.	-1122.
S_J-S_o		cal/°K/gm HE	0.1464	0.07526	0.05367	0.00423	0.06991	0.05091	0.00652
Composition of Product Mixture	CF_2	10^{-3}mole/gm HE	-	*	*	*	*	*	*
	CF_3		-	*	*	*	*	*	*
	CF_4		-	1.050	1.987	2.808	1.030	1.970	2.808
	CH_2F_2		-	*	*	-	*	*	-
	CH_3F		-	*	*	-	*	*	-
	CH_4		*	*	*	-	*	*	-
	CHF_3		-	*	*	-	*	*	-
	CO		1.005	0.2629	0.1865	0.06090	0.4609	0.3702	0.1847
	CO_2		10.06	10.72	10.97	11.20	10.64	10.89	11.14
	COF_2		-	*	*	*	*	*	*
	F		-	*	*	*	*	*	*
	F_2		-	*	*	*	*	*	*
	H		-	*	*	-	*	*	-
	H_2		-	*	*	-	*	*	-
	H_2O		7.036	4.264	1.966	-	4.221	1.932	-
	HF		-	0.1257	0.08100	-	0.2069	0.1476	-
	N_2		7.038	6.490	6.022	5.616	6.490	6.021	5.616
	N_2O		-	*	*	*	*	*	*
	NH_3		*	*	*	-	*	*	-
	NO		-	*	*	*	*	*	*
	NO_2		-	*	*	*	*	*	*
	O		-	*	*	*	*	*	*
	O_2		-	*	*	*	*	*	*
	OH		-	*	*	-	*	*	-
	C(graphite)		17.09	13.93	10.95	8.394	13.83	10.85	8.332
Σ moles gas		10^{-3}moles/gm HE	25.14	22.91	21.21	19.69	23.05	21.34	19.49
V_c		cc/mole	14.97	15.58	17.19	18.23	15.15	16.70	17.73
V_s		cc/mole	3.953	3.833	3.866	3.824	3.886	3.925	3.902

*Mole fraction in gas mixture less than 10^{-4}

TABLE 8. COMPUTED DETONATION PROPERTIES FOR FLUORINATED TETRYLS

Property		Units	Tetryl	MFT	DFT	MFT	DFT
(Parameter Type)			RDX	RDX	RDX	TNT	TNT
ΔH_f		kcal/mole	+4.67	-42.	-87.	-42.	-87.
ρ_o		gms/cc	1.73	1.84	1.92	1.84	1.92
D		mm/μsec	7.817	8.031	8.129	7.596	7.599
P_J		megb	0.2644	0.2927	0.3065	0.2765	0.2852
T_J		°K	2971.	2734.	2543.	2964.	2831.
ρ_J		gms/cc	2.307	2.442	2.532	2.488	2.585
γ			2.999	3.055	3.139	2.839	2.887
E_J-E_o		cal/gm HE	456.7	468.8	460.9	467.8	456.7
ΔE_{chem}		cal/gm HE	-1422.	-1355.	-1295.	-1351.	-1292.
S_J-S_o		cal/°K/gm HE	+0.07156	+0.02059	-0.01841	+0.01466	-0.01905
Composition of Product Mixture	CF_2	10^{-3}moles/gm HE	-	*	*	*	*
	CF_3		-	*	*	*	*
	CF_4		-	0.7902	1.536	0.7684	1.520
	CH_2F_2		-	*	*	*	*
	CH_3F		-	*	*	*	*
	CH_4		*	*	*	*	*
	CHF_3		-	*	*	*	*
	CO		0.7063	0.2461	0.09655	0.4537	0.2502
	CO_2		9.225	9.738	10.02	9.657	9.961
	COF_2		-	*	*	*	*
	F		-	*	*	*	*
	F_2		-	*	*	*	*
	H		-	*	*	*	*
	H_2		-	*	*	*	*
	H_2O		8.705	6.496	4.619	6.449	4.585
	HF		-	0.1157	0.04515	0.2028	0.1104
	N_2		8.706	8.193	7.737	8.191	7.736
	N_2O		-	*	*	*	*
	NH_3		*	*	*	*	*
	NO		-	*	*	*	*
	NO_2		-	*	*	*	*
	O		-	*	*	*	*
	O_2		-	*	*	*	*
	OH		-	*	*	*	*
	C(graphite)		14.45	12.17	10.01	12.06	9.932
Σ moles gas		10^{-3}moles/gm HE	27.34	25.58	24.06	25.73	24.16
V_g		cc/mole	13.82	14.22	14.87	13.84	14.45
V_s		cc/mole	3.846	3.760	3.718	3.811	3.783

*Mole fraction in gas mixture less than 10^{-4}

TABLE 9. COMPUTED DETONATION PROPERTIES FOR FLUORINATED TNT's AND DATB

Property	Units	TNT	MFTNT	DFTNB	MFTNT	DFTNT	DATB	FDATB	FDATB
(Parameter Type)		TNT	TNT	TNT	RDX	RDX	TNT	TNT	RDX
ΔH_f	kcal/mole	-17.81	-64.	-109.	-64.	-109.	-29.23	-76.	-76.
ρ_o	gms/cc	1.651	1.79	1.88	1.79	1.88	1.837	1.97	1.97
D	mm/μsec	7.000	7.204	7.208	7.586	7.695	7.661	7.823	8.498
P_J	megb	0.2071	0.2383	0.2466	0.2520	0.2644	0.2679	0.2953	0.3256
T_J	°K	2884.	2704.	2568.	2529.	2339.	2373.	2151.	1843.
ρ_J	gms/cc	2.219	2.408	2.515	2.367	2.466	2.444	2.609	2.555
Y		2.907	2.898	2.961	3.104	3.210	3.025	3.082	3.370
E_J-E_o	cal/gm HE	383.7	408.1	395.7	408.2	399.2	432.9	438.8	451.9
ΔE_{chem}	cal/gm HE	-1280.	-1209.	-1144.	-1211.	-1146.	-1165.	-1096.	-1096.
S_J-S_o	cal/°K/gm HE	+0.09679	+0.03903	-0.00105	0.04574	0.000085	-0.1204	-0.1789	-0.1904
Composition of Product Mixture CF_2	10^{-3}moles/gm HE	-	*	*	*	*	-	*	*
CF_3		-	*	*	*	*	-	*	*
CF_4		-	0.9419	1.862	0.9694	1.883	-	0.9507	0.9564
CH_2F_2		-	*	*	*	*	-	*	*
CH_3F		-	*	*	*	*	-	*	*
CH_4		*	*	*	*	*	*	*	*
CHF_3		-	*	*	*	*	-	*	*
CO		0.8523	0.3233	0.1582	0.1941	0.06625	0.1058	0.02596	0.003553
CO_2		7.282	8.077	8.511	8.113	8.536	7.145	7.653	7.658
COF_2		-	*	*	*	*	-	*	*
F		-	*	*	*	*	-	*	*
F_2		-	*	*	*	*	-	*	*
H		-	*	*	*	*	-	*	*
H_2		-	*	*	*	*	-	*	*
H_2O		11.00	7.999	5.623	8.057	5.666	10.28	7.645	7.657
HF		-	0.3116	0.1515	0.2018	0.06982	-	0.02670	0.004118
N_2		6.602	6.118	5.700	6.119	5.701	10.28	9.574	9.574
N_2O		-	*	*	*	*	-	*	*
NH_3		0.003797	*	*	*	*	*	*	*
NO		-	*	*	*	*	-	*	*
NO_2		-	*	*	*	*	-	*	*
O		-	*	*	*	*	-	*	*
O_2		-	*	*	*	*	-	*	*
OH		-	*	*	*	*	-	*	*
C(graphite)		22.68	19.21	16.07	19.28	16.12	17.43	14.35	14.36
Σ moles gas	10^{-3}moles/gm HE	25.74	23.77	22.01	23.66	21.92	27.61	25.88	25.85
V_g	cc/mole	13.96	14.31	15.23	14.71	15.69	12.32	12.74	13.11
V_s	cc/mole	4.028	3.913	3.881	3.866	3.819	3.811	3.731	3.64

*Mole fraction in gas mixture less than 10^{-4}

TABLE 10. COMPUTED DETONATION PROPERTIES FOR RING-FLUORINATED TNBTF's

Property		Units	TNBTF	MFTNBTF	DFTNBTF	TNBTF	MFTNBTF	DFTNBTF
(Parameter Type)			RDX	RDX	RDX	TNT	TNT	TNT
ΔH_f		kcal/mole	-171.	-216.	-261.	-171.	-216.	-261.
ρ_o		gms/cc	1.9	2.0	2.1	1.9	2.0	2.1
D		mm/μsec	7.506	7.696	7.911	6.956	7.010	7.070
P_J		megb	0.2507	0.2707	0.2931	0.2303	0.2425	0.2557
T_J		°K	2115.	1909.	1699.	2372.	2233.	2094.
ρ_J		gms/cc	2.481	2.593	2.703	2.535	2.655	2.776
γ			3.271	3.375	3.485	2.992	3.052	3.104
E_J-E_o		cal/gm HE	369.2	369.7	371.9	362.8	357.5	354.6
ΔE_{chem}		cal/gm HE	-1027.	-979.4	-936.8	-1026.	-979.0	-936.6
S_J-S_o		cal/°K/gm HE	-0.04528	-0.09342	-0.1458	-0.04165	-0.08129	-0.1228
Composition of Product Mixture	CF_2	10^{-3}mole/gm HE	*	*	*	*	*	*
	CF_3		*	*	*	*	*	*
	CF_4		2.660	3.342	3.942	2.646	3.337	3.942
	CH_2F_2		*	*	-	*	*	-
	CH_3F		*	*	-	*	*	-
	CH_4		*	*	-	*	*	-
	CHF_3		*	*	-	*	*	-
	CO		0.02367	0.004256	*	0.08013	0.03019	0.009924
	CO_2		8.889	9.193	9.461	8.876	9.186	9.456
	COF_2		*	*	*	*	*	*
	F		*	*	*	*	*	*
	F_2		*	*	*	*	*	*
	H		*	*	-	*	*	-
	H_2		*	*	-	*	*	-
	H_2O		3.542	1.670	-	3.511	1.659	-
	HF		0.03083	0.004286		0.08948	0.02495	-
	N_2		5.336	5.015	4.731	5.336	5.015	4.731
	N_2O		*	*	*	*	*	*
	NH_3		*	*	-	*	*	-
	NO		*	*	*	*	*	*
	NO_2		*	*	*	*	*	*
	O		*	*	*	*	*	*
	O_2		*	*	*	*	*	*
	OH		*	*	-	*	*	-
	C(graphite)		13.33	10.86	8.672	13.30	10.85	8.668
Σ moles gas		10^{-3}moles/gm HE	20.48	19.23	18.13	20.54	19.25	18.14
V_g		cc/mole	17.17	17.92	18.63	16.67	17.38	18.02
V_s		cc/mole	3.849	3.785	3.719	3.924	3.879	3.834

*Mole fraction in gas mixture less than 10^{-4}

TABLE 11. COMPUTED DETONATION PROPERTIES FOR FDNP/FTNM MIXTURES
(Using RDX-Type Parameters)

Property		Units	FDNP	FDNP/FTNM 55.0/45.0	FDNP/FTNM 50.3/49.7	FDNP/FTNM 45.0/55.0	FTNM
ΔH_f		cal/gm	-528.7	-390.1	-375.6	-359.3	-220.7
ΔH_f		kcal/mole	-80.4	-	-	-	-37.3
ρ_o		gms/cc	1.35	1.4469	1.4578	1.4703	1.586
D		mm/μsec	6.848	7.258	7.211	7.108	6.089
P_J		megb	0.1809	0.2160	0.2165	0.2103	0.1416
T_J		°K	2817.	3417.	3614.	3414.	1289.
ρ_J		gms/cc	1.890	2.019	2.041	2.051	2.089
γ			2.500	2.528	2.501	2.532	3.152
E_J-E_o		cal/gm HE	457.5	505.7	506.9	484.0	257.1
ΔE_{chem}		cal/gm HE	-1253.	-1455.	-1508.	-1409.	-531.7
S_J-S_o		cal/°K/gm HE	-0.02247	+0.05126	+0.04768	+0.02622	-0.3784
Composition of Product Mixture	CF_2	10^{-3}moles/gm HE	*	*	*	*	*
	CF_3		*	*	*	*	*
	CF_4		0.8976	1.129	1.084	1.122	1.479
	CH_2F_2		*	*	*	*	-
	CH_3F		*	*	*	*	-
	CH_4		*	*	*	*	-
	CHF_3		*	*	*	*	-
	CO		1.115	2.480	0.2557	0.02987	*
	CO_2		5.128	9.901	11.52	10.98	4.437
	COF_2		*	*	*	*	*
	F		0.003654	0.01543	0.08283	0.1190	*
	F_2		*	*	0.005129	0.01535	*
	H		*	*	*	*	-
	H_2		0.008791	0.007511	*	*	-
	H_2O		14.93	8.153	7.359	6.610	-
	HF		2.981	1.743	1.816	1.573	-
	N_2		6.572	7.605	7.664	7.587	8.635
	N_2O		*	*	0.008053	0.03166	*
	NH_3		0.005459	0.004899	*	*	-
	NO		*	0.003636	0.08568	0.3190	0.003748
	NO_2		*	*	0.006171	0.1230	0.4710
	O		*	*	*	*	*
	O_2		*	*	0.05269	1.082	12.84
	OH		*	*	*	*	-
	C(graphite)		12.58	0.	0.	0.	0.
Σ moles gas		10^{-3}moles/gm HE	31.64	31.05	29.94	29.59	27.87
V_g		cc/mole	15.08	15.95	16.36	16.48	17.18
V_s		cc/mole	4.128	4.021	4.029	4.042	4.228

*Mole fraction in gas mixture less than 10^{-4}

TABLE 12. LITERATURE VALUES FOR DETONATION VELOCITIES

		NOL (Calculated)		Literature		
HE	ρ_o (gm/cc)	ΔH_f (Kcal/mole)	D[RDX/TNT] (mm/μsec)	Ref.	ΔH_f (Kcal/mole)	D (mm/μsec)
DFTNB	1.695	-103.	6.924	a		7.190
	1.768	-103.	7.155	a		7.415
	1.841	-103.	7.404	a		7.636
	1.855(extrap)			a		7.750
	1.84			b		7.474
	1.855			c(Expt)		7.618
	1.873			c(Calc)	-51.3	7.618
	1.8564	-103.	7.459/7.009			
DFTNBTF	1.937			c(Calc)	(sic)225.0	6.799
	2.1	-261.	7.911/7.070			
MFTN3	1.512	-58.	6.659	a		6.650
	1.615	-58.	6.936	a		7.050
	1.802	-58.	7.526	a		7.515
	1.80			b		7.182
	1.83			c(Expt)		7.655
	1.802			c(Calc)	-47.1	7.766
	1.8383	-58.	7.657/7.242			
MFTNBTF	1.887			c(Calc)	-184.2	7.050
	2.0	-216.	7.696/7.010			
TFTNB	1.964	-148.	7.603	a		7.502
	1.920			c(Calc)	-135.1	7.085
	1.9477	-148.	7.541/6.982			
TNBTF	1.82			a		7.170
	1.82			b		6.919
	1.805			c(Expt)		7.185
	1.816			c(Calc)	-142.2	7.249
	1.9	-171.	7.506/6.956			

References:
a. Denver Research Institute (Ref. 1)
b. Picatinny Arsenal (Ref. 13)
c. Amcel Propulsion Company (Ref. 14)

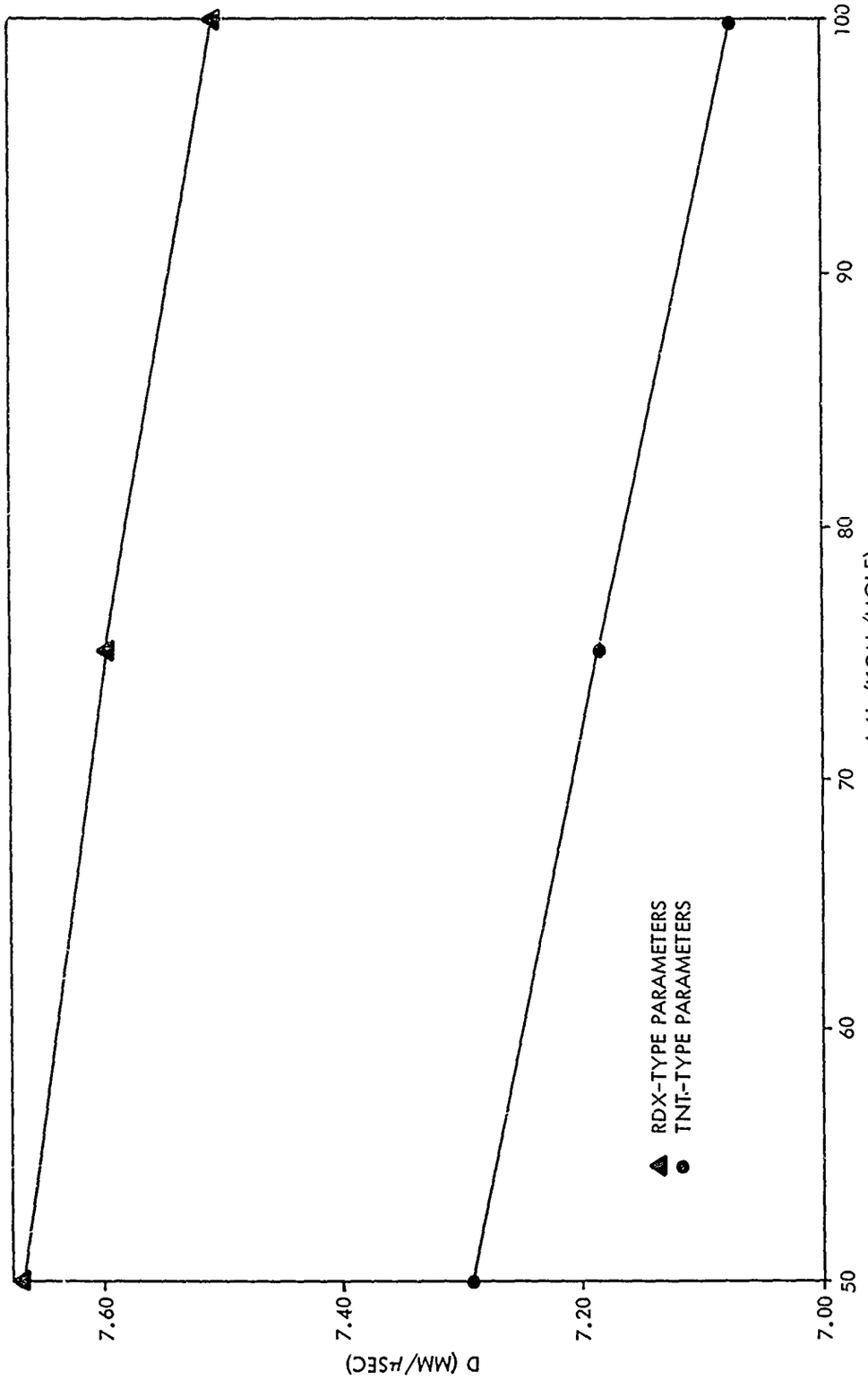


FIG. 1 COMPUTED D FOR MFTNT, VARYING ΔH_f AND EQUATION OF STATE PARAMETERS

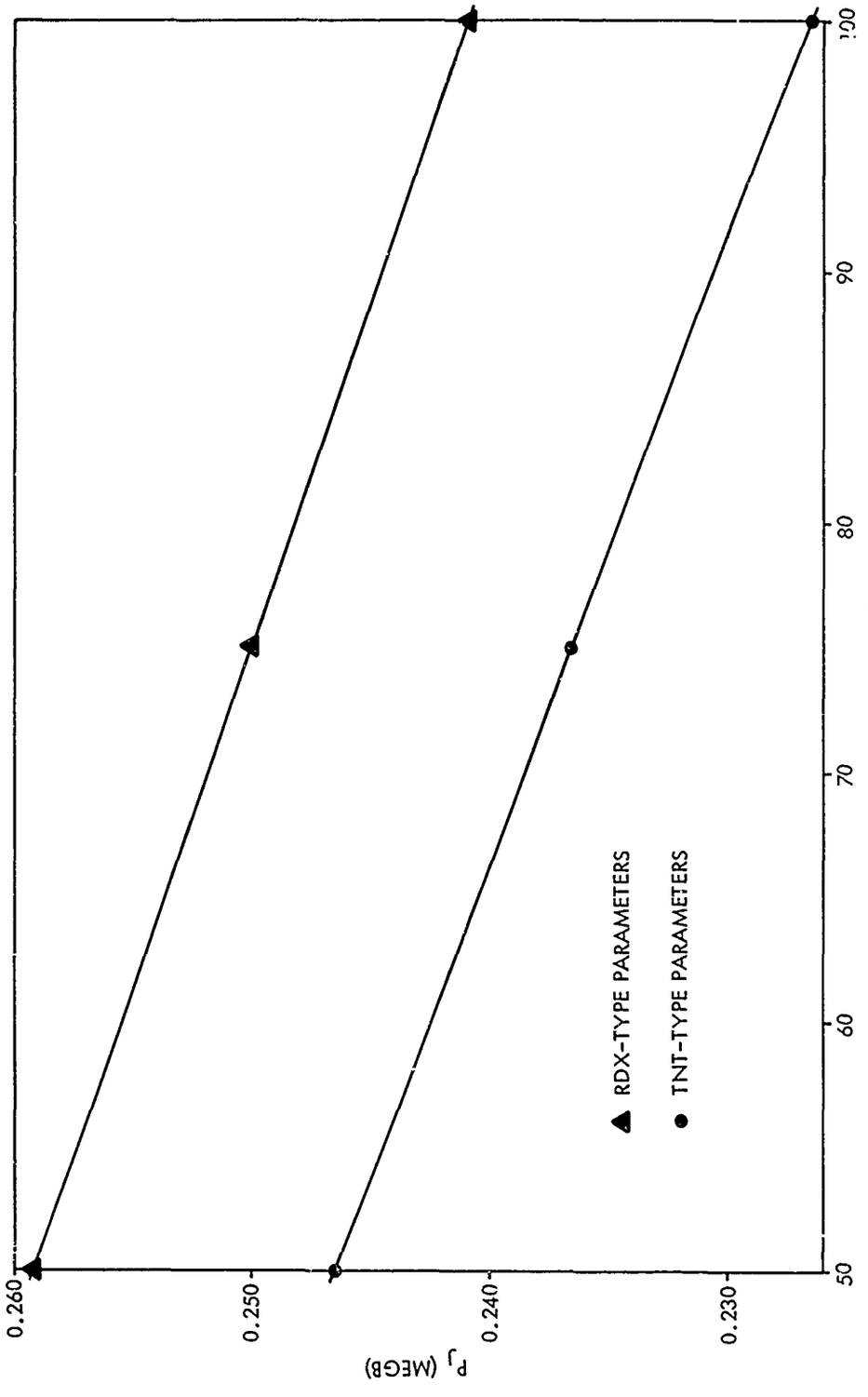


FIG. 2 COMPUTED P_J FOR MFTNT, VARYING ΔH_f AND EQUATION OF STATE PARAMETERS

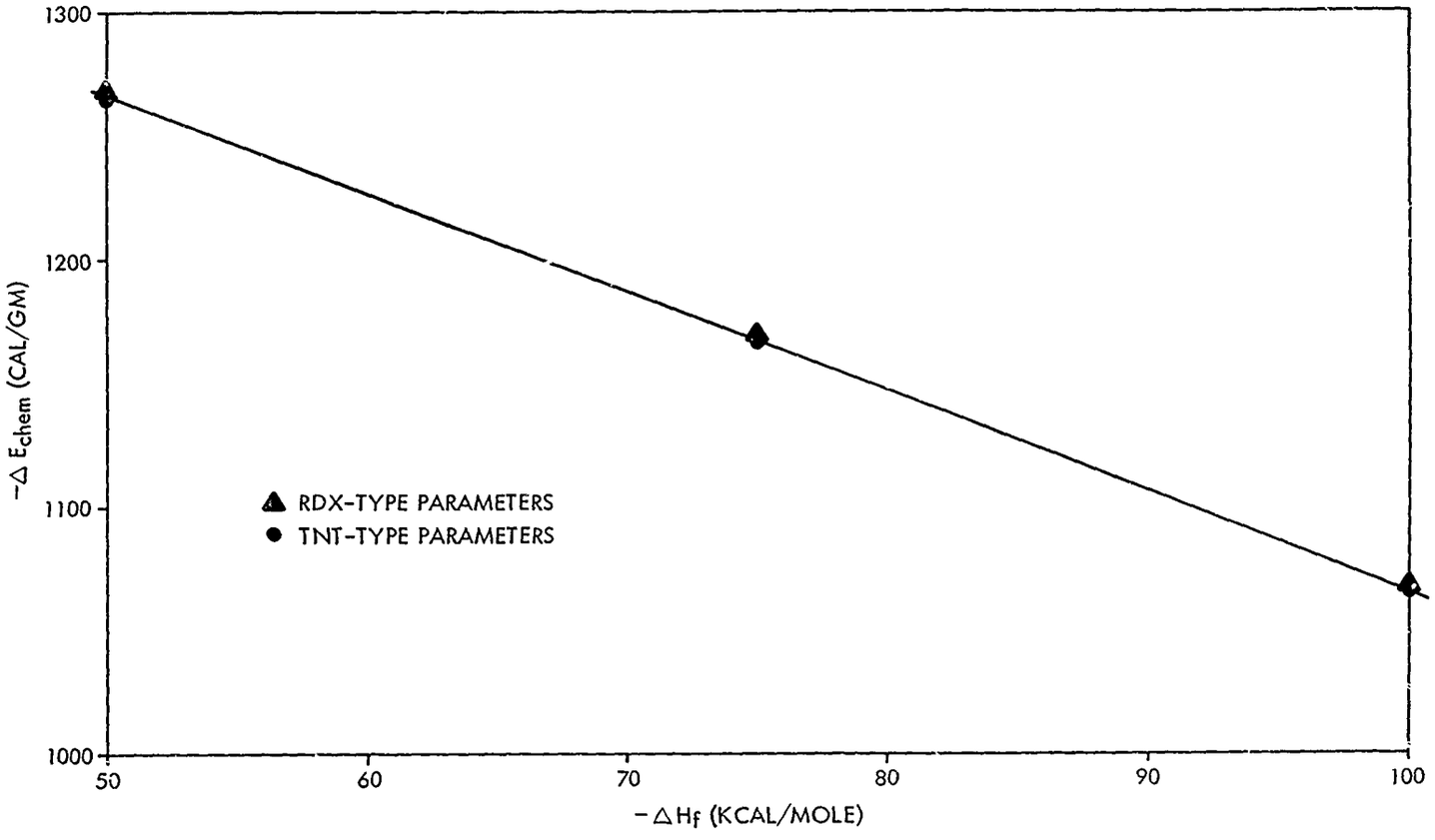


FIG. 3 COMPUTED ΔE_{chem} FOR MFTNT, VARYING ΔH_f AND EQUATION OF STATE PARAMETERS

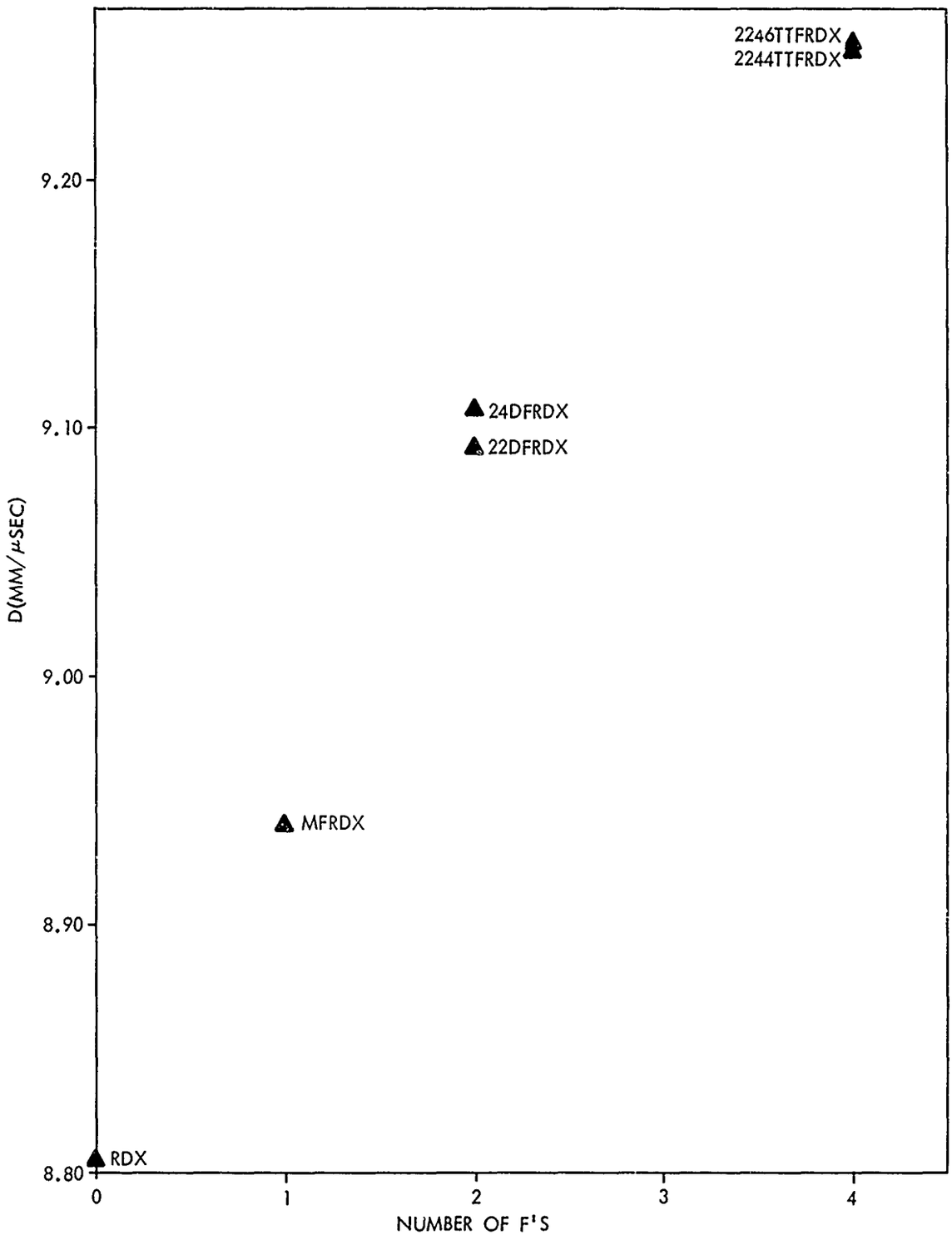


FIG. 4 COMPUTED DETONATION VELOCITY VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED RDX'S

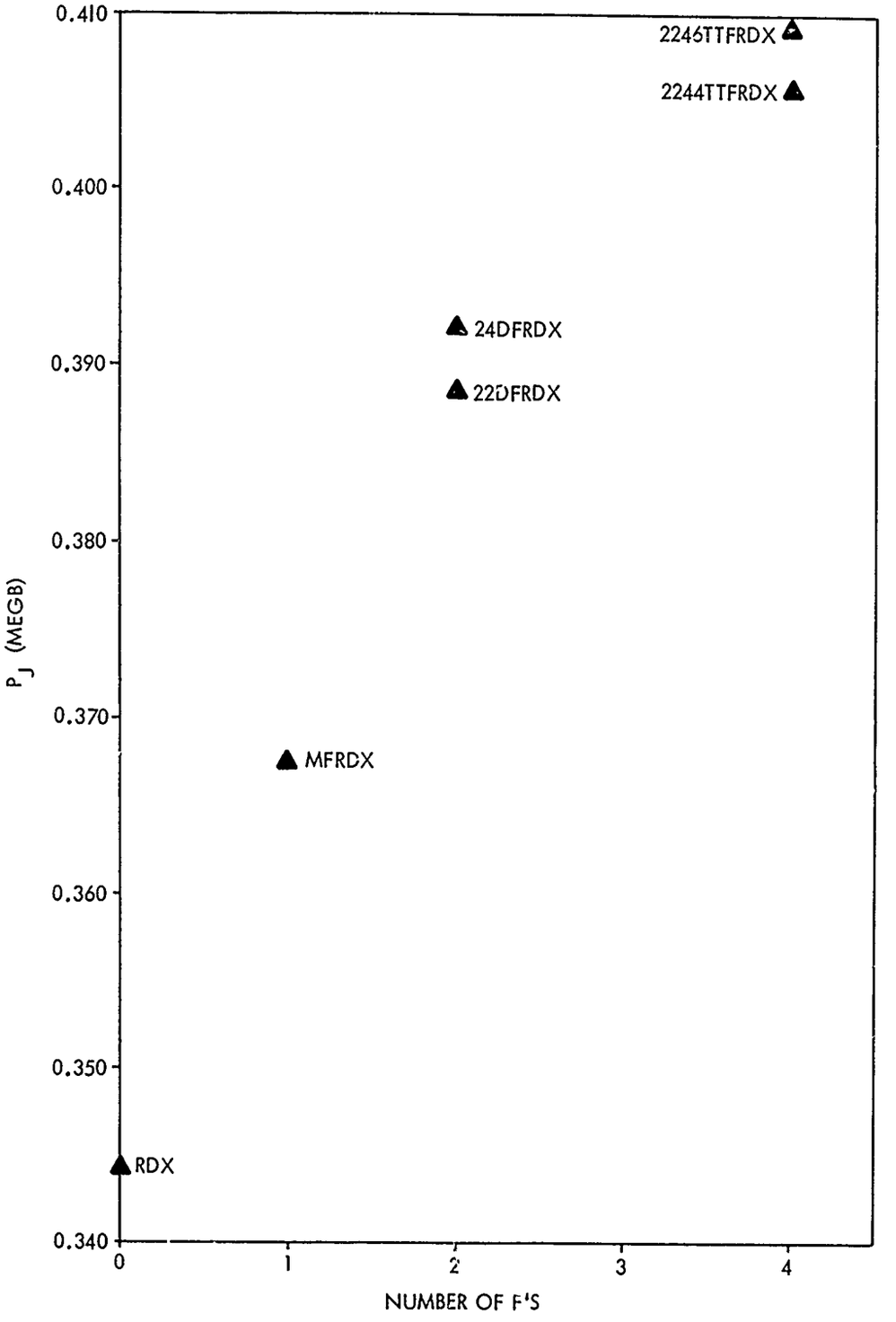


FIG. 5 COMPUTED CJ PRESSURE VS NUMBER OF FLUORINE ATOMS FOR FLUORINATED RDX'S

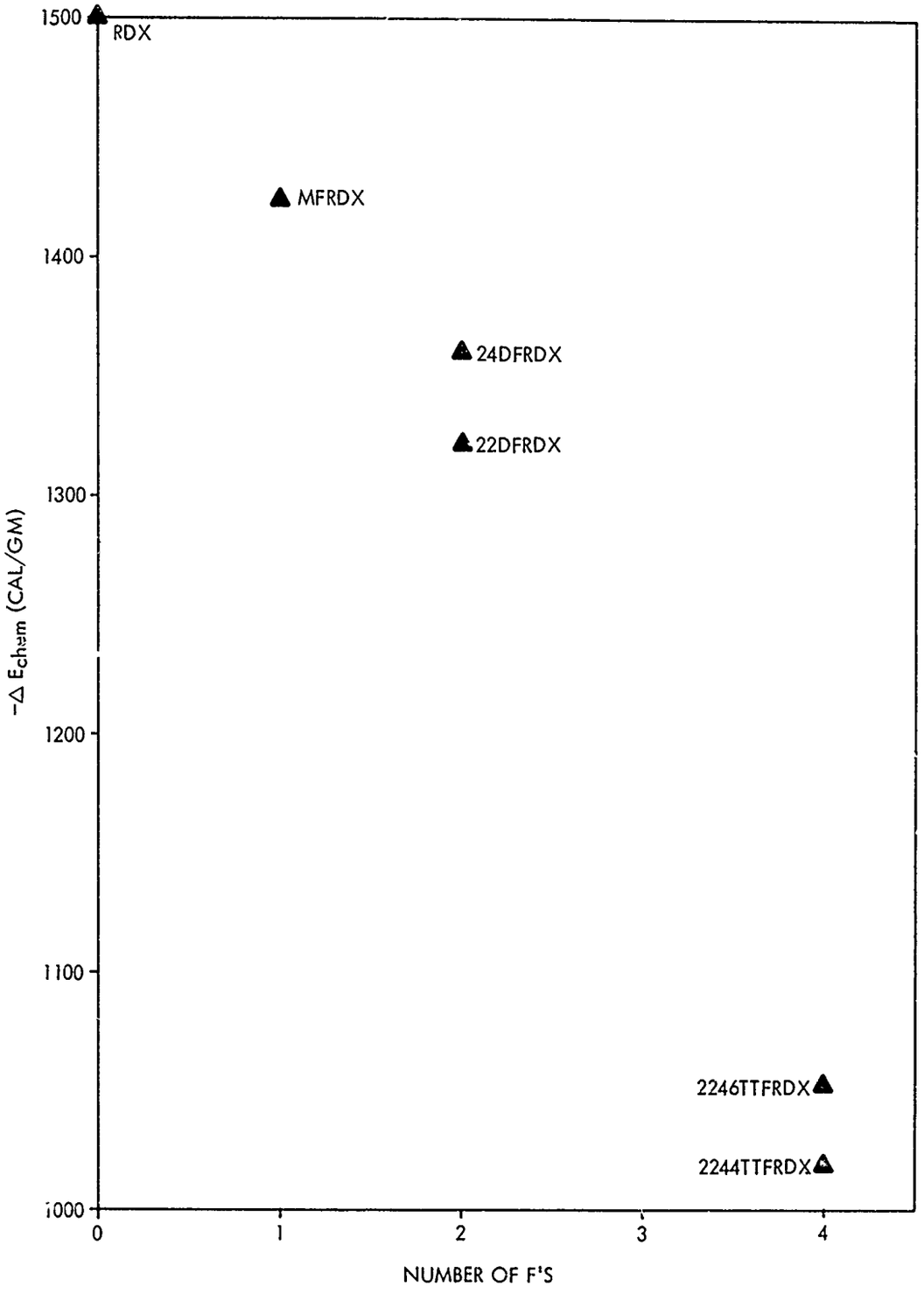


FIG. 6 COMPUTED CHEMICAL ENERGY VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED RDX'S

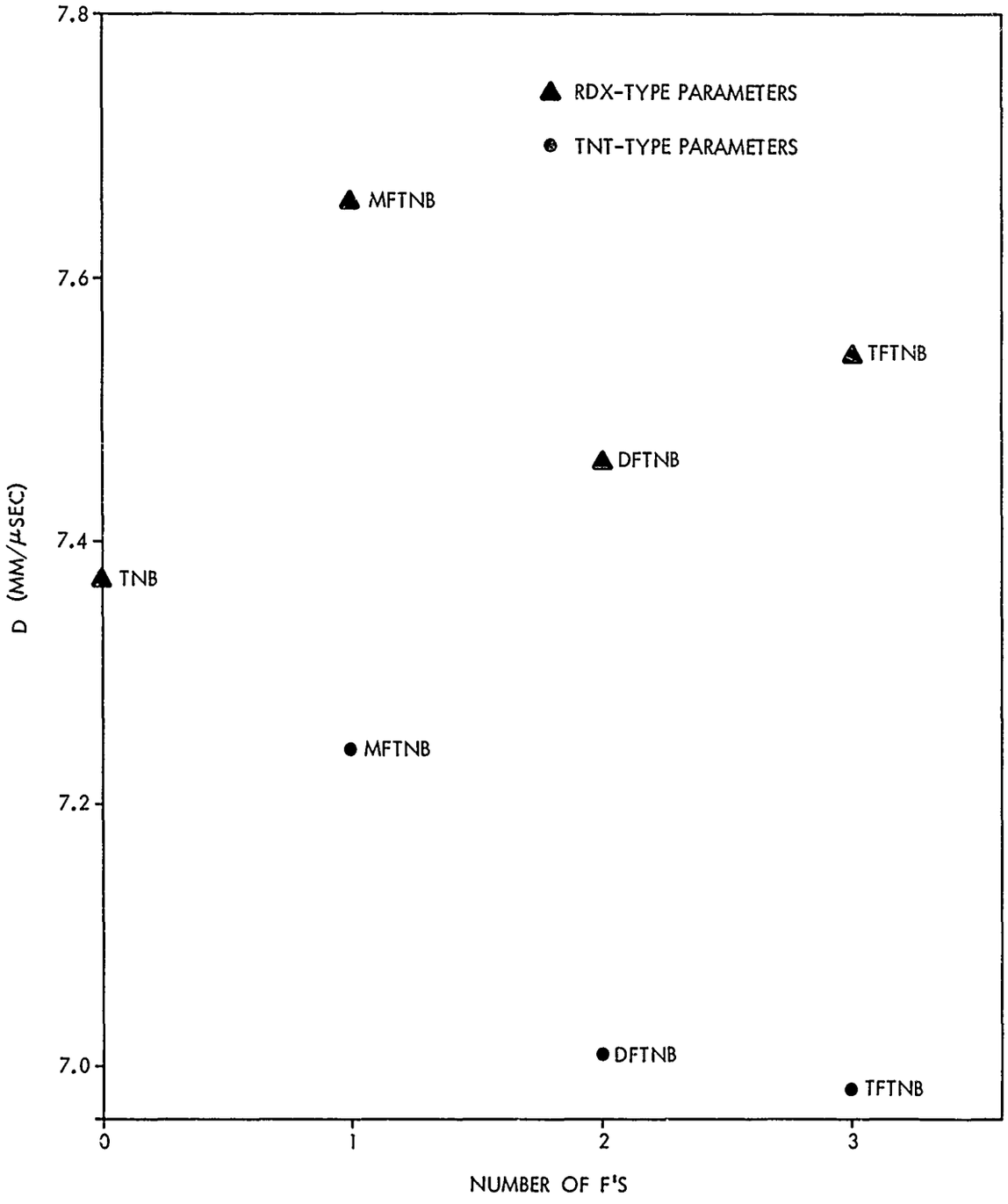


FIG. 7 COMPUTED DETONATION VELOCITY VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED TNB'S

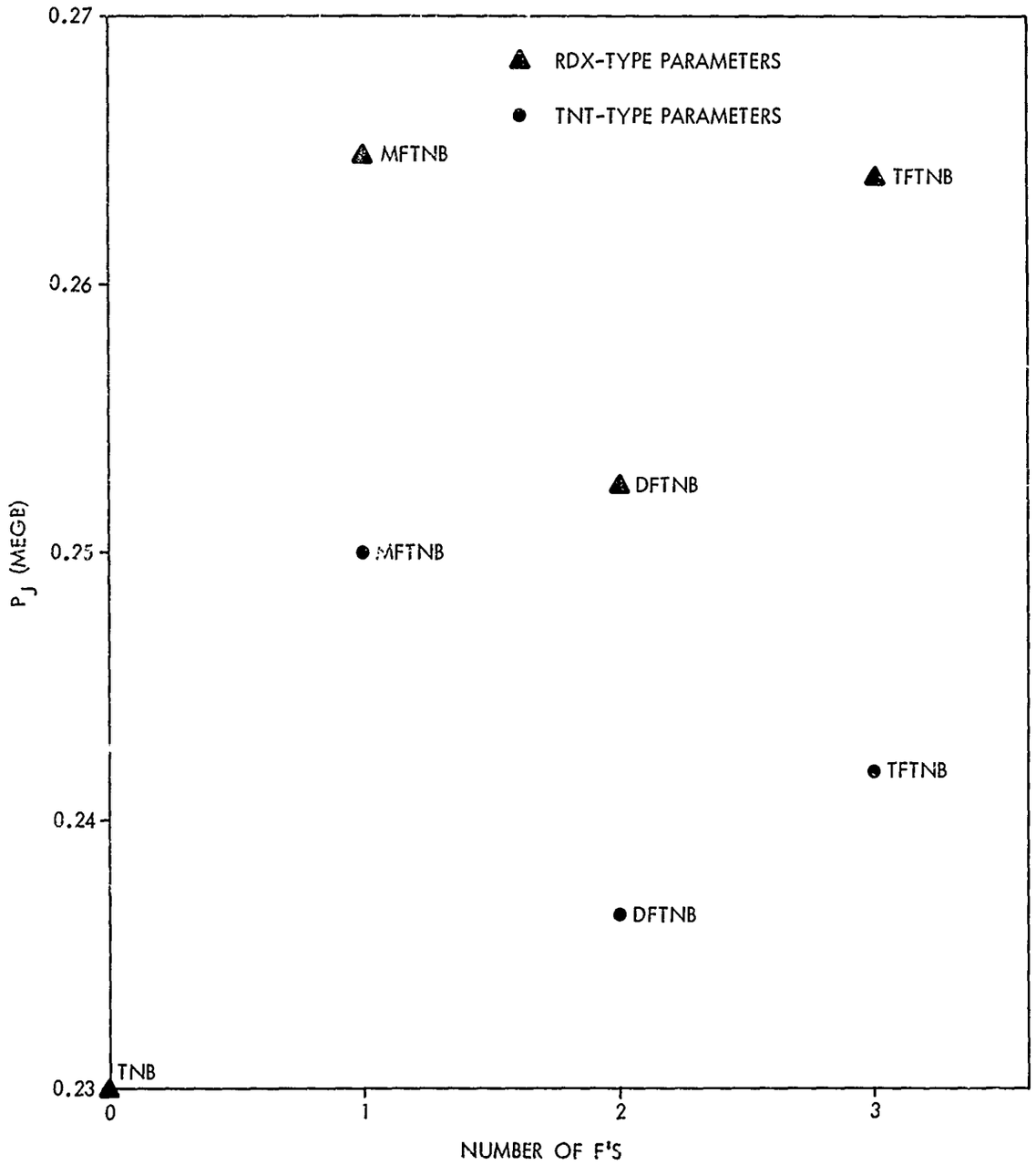


FIG. 8 COMPUTED CJ PRESSURE VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED TNB'S

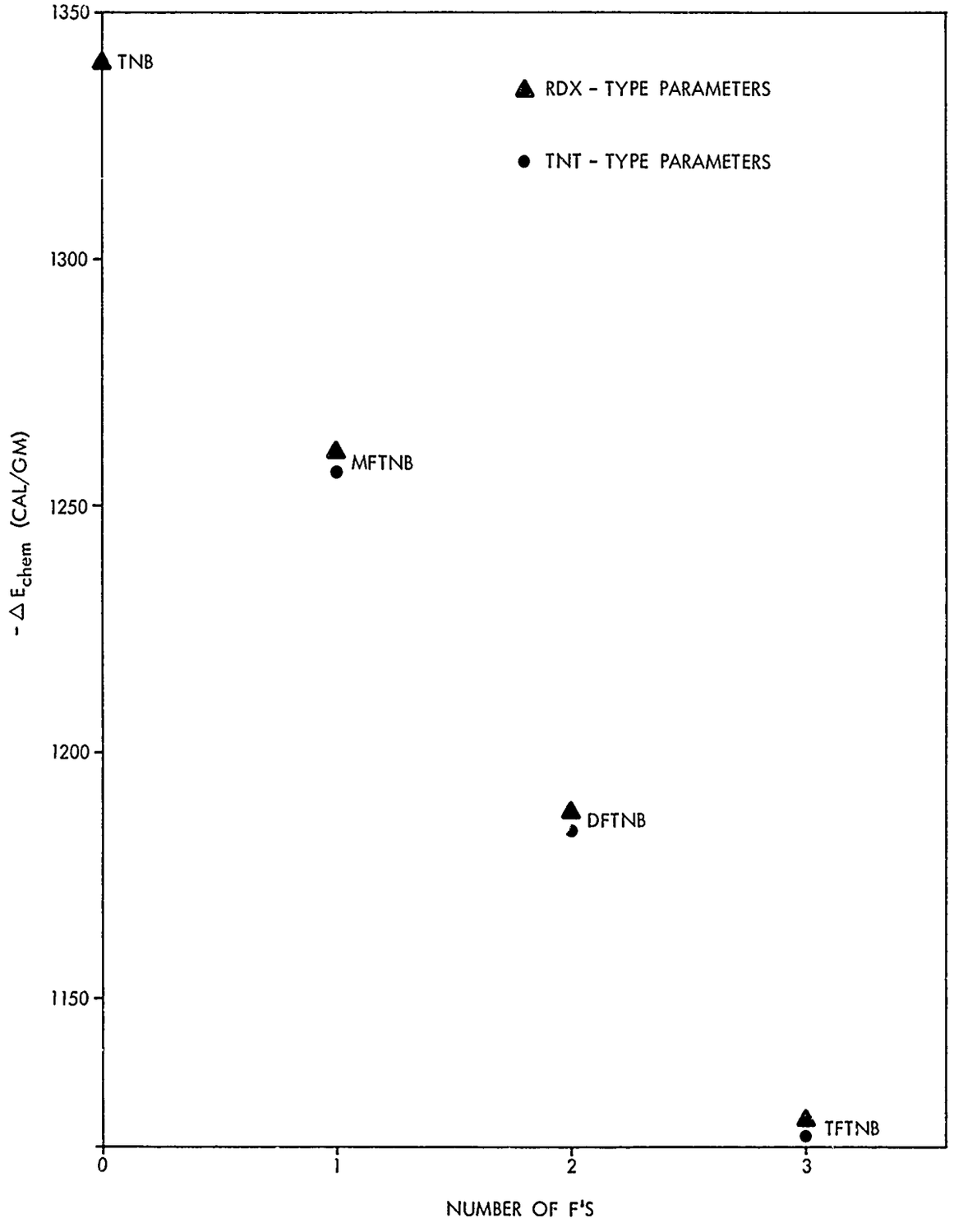


FIG. 9 COMPUTED CHEMICAL ENERGY VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED TNB'S

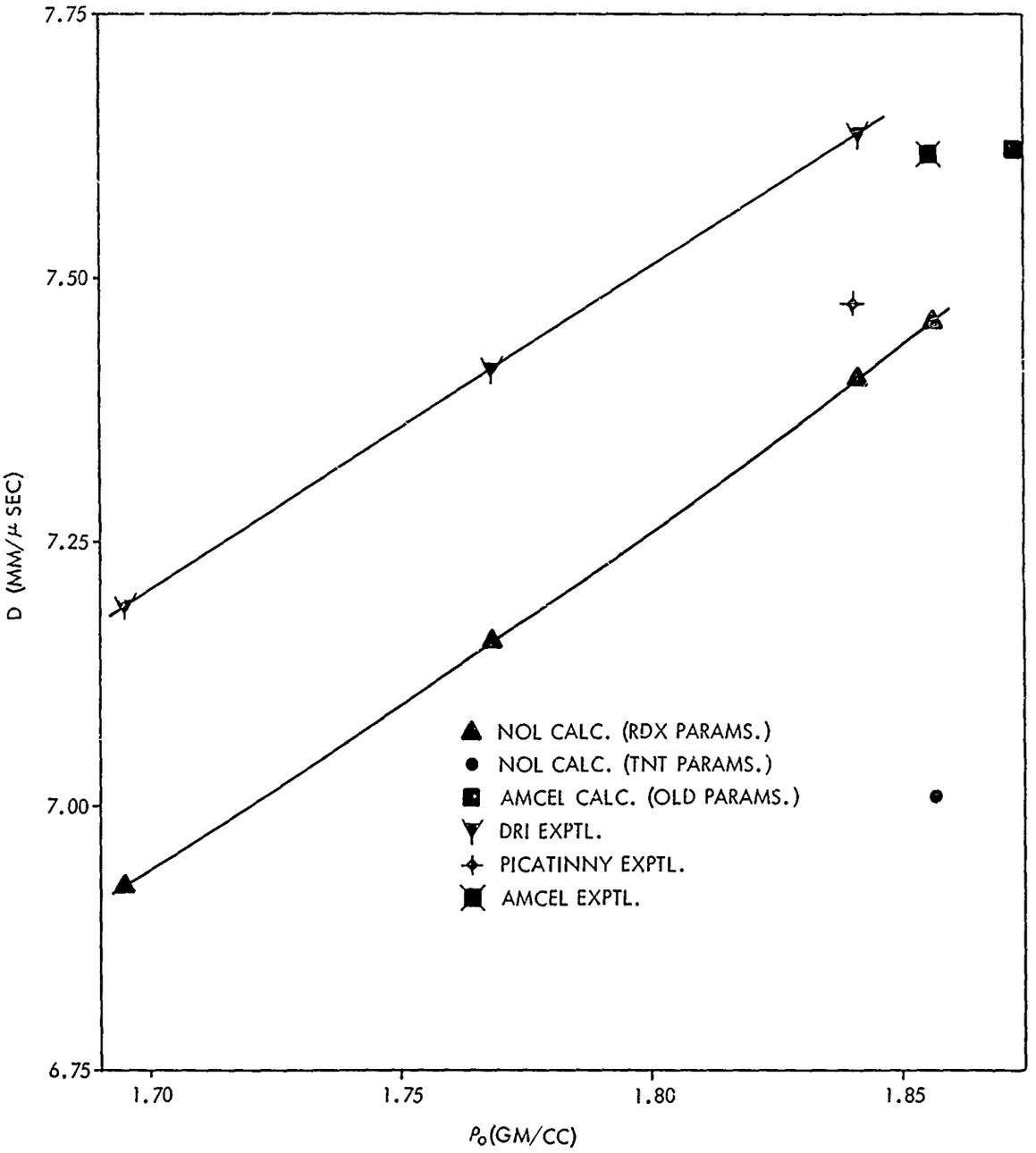


FIG. 10. DETONATION VELOCITIES FOR DFTNB, FROM NOL AND OTHER SOURCES

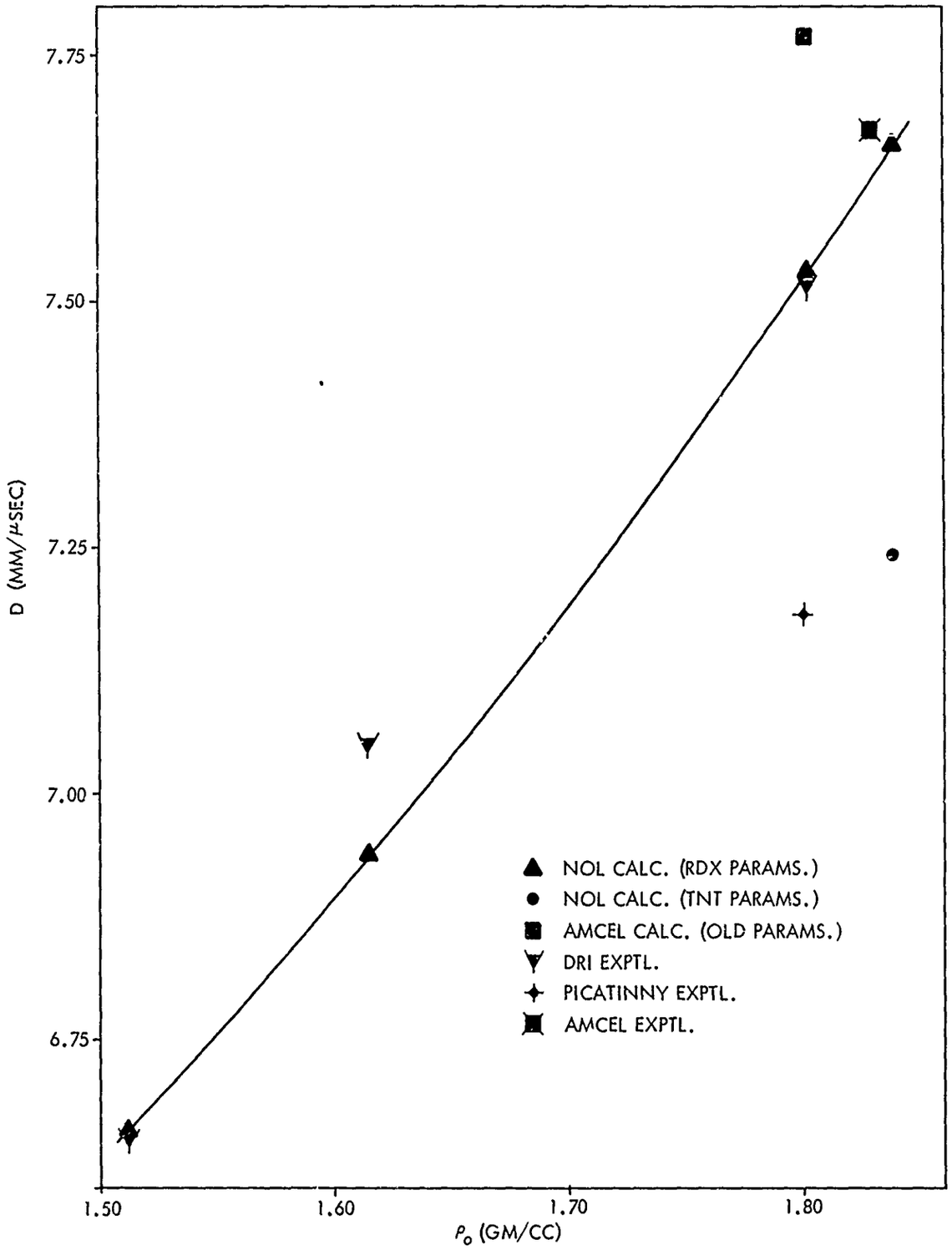


FIG. 11. DETONATION VELOCITIES FOR MFTNB, FROM NOL AND OTHER SOURCES

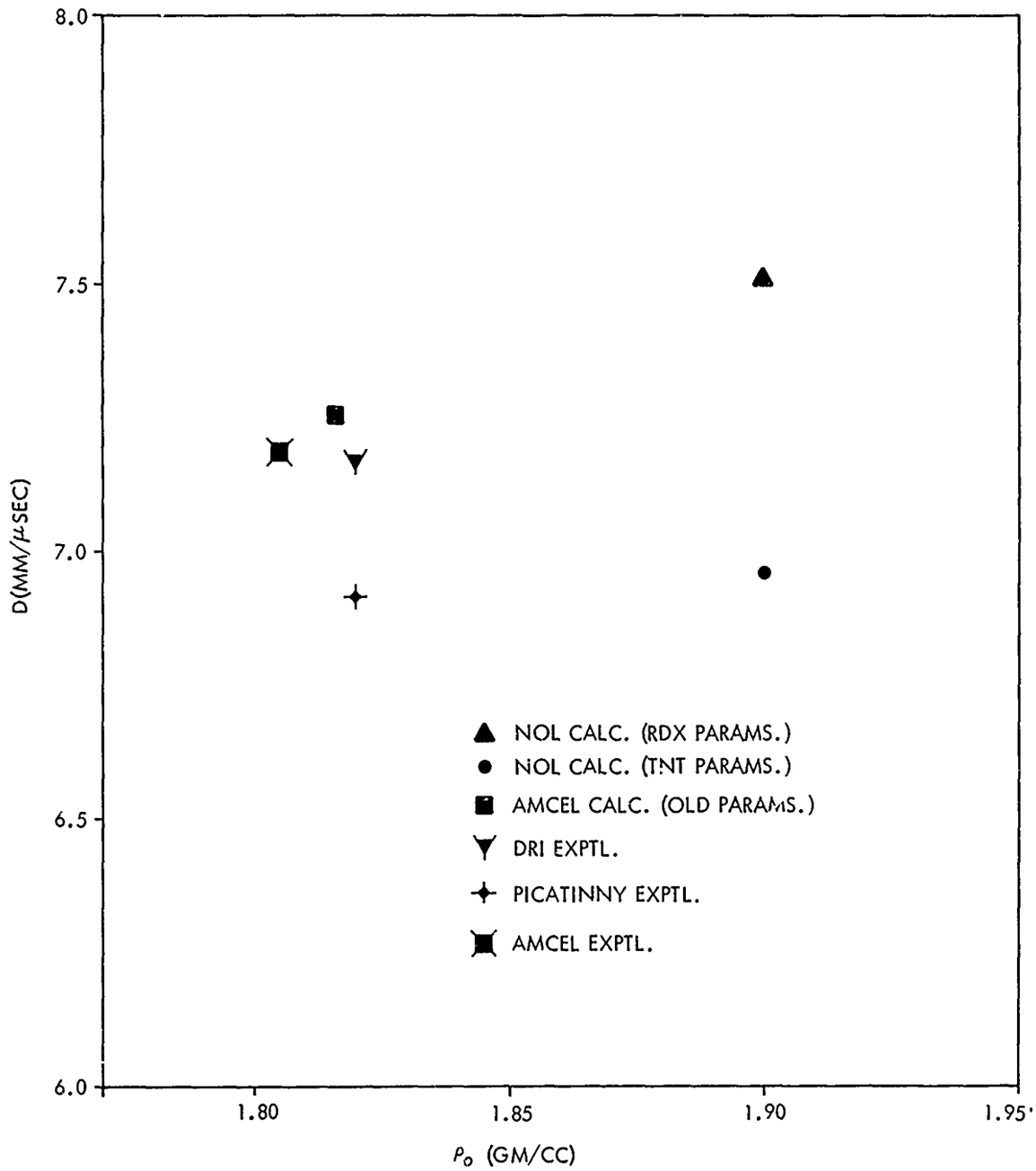


FIG. 12. DETONATION VELOCITIES FOR TNBTF, FROM NOL AND OTHER SOURCES

APPENDIX

ESTIMATION OF HEATS OF FORMATION (ΔH_f)

		ΔH_f (kcal/mole)		Reference
MFTNB				
	$C_6H_5F(\ell)$	-34.8		15
	$C_6H_6(\ell)$	+11.72		16
	(Fluoro-)	-46.5	(Difference)	
	TNB(s)	-11.4		4
	MFTNB(s)	-57.9	(Sum)	
DFTNB				
	$m\text{-}C_6H_4F_2(\ell)$	-79.64		17
	$C_6H_6(\ell)$	+11.72		16
	(Difluoro-)	-91.36	(Difference)	
	TNB(s)	-11.40		4
	DFTNB(s)	-102.76	(Sum)	
TFTNB				
	$m\text{-}C_6H_4F_2(\ell)$	-79.64		17
	$C_6H_5F(\ell)$	-34.8		15
	(Fluoro-)	-44.8	(Difference)	
	DFTNB(s)	-103.0		
	TFTNB(s)	-148.0	(Sum)	
TNBTF				
	TNB(s)	-11.40		4
	$C_6H_6(\ell)$	+11.72		16
	(Trinitro)	-23.12	(Difference)	
	$C_6H_5CF_3(\ell)$	-147.8		15
	TNBTF(s)	-170.9	(Sum)	
MFTNBTF				
	TNB(s)	-11.40		4
	$C_6H_6(\ell)$	+11.72		16
	(Trinitro-)	-23.12	(Difference)	
	$m\text{-}FC_6H_4CF_3(\ell)$	-193.2		18
	MFTNBTF(s)	-216.3	(Sum)	

APPENDIX Contd

		ΔH_f (kcal/mole)		Reference
DFTNBTF				
	MFTNBTF(s)	-216.3	(Estimated)	
	TNBTF(s)	-170.9	(Estimated)	
	(Fluoro-)	-45.4	(Difference)	
	MFTNBTF(s)	-216.3		
	DFTNBTF(s)	-261.7	(Sum)	
MFTNT				
	TNT(s)	-17.81		4
	$C_6H_5CH_3(\ell)$	+2.867		16
	(Trinitro-)	-20.68	(Difference)	
	$p\text{-}FC_6H_4CH_3(\ell)$	-43.43		17
	MFTNT(s)	-64.11	(Sum)	
DFTNT				
	MFTNT(s)	-64	(Estimated)	
	MFTNB(s)	-58	(Estimated)	
	(Methyl-)	-6	(Difference)	
	DFTNB(s)	-103	(Estimated)	
	DFTNT(s)	-109	(Sum)	
FDATB				
	$C_6H_5F(\ell)$	-34.8		15
	$C_6H_6(\ell)$	+11.7		16
	(Fluoro-)	-46.5	(Difference)	
	DATB(s)	-29.2		4
	FDATB(s)	-75.7	(Sum)	
MFRDX				
	RDX	+14.71		4
	*	-40.4		(See Ref. 18)
	MFRDX	-25.7	(Sum)	

*Heats of formation of the fluorinated RDX's were estimated by using the increments for substitution of a fluorine atom for a hydrogen atom in aliphatic hydrocarbons given by Good et al in reference 18. The increments vary with the number of other fluorines attached to the same carbon atom and are therefore listed separately in this table.

APPENDIX Contd

		ΔH_f (kcal/mole)		Reference
22DFRDX				
	RDX	+14.71		4
	*	-40.4		(See Ref. 18)
	MFRDX	-25.7	(Sum)	
22DFRDX				
	RDX	+14.71		4
	*	-90.4		(See Ref. 18)
	22DFRDX	-75.7	(Sum)	
24DFRDX				
	RDX	+14.71		4
	*	2(-40.4)		(See Ref. 18)
	24DFRDX	-66.1	(Sum)	
224TFRDX				
	RDX	+14.71		4
	*	-90.4 -40.4		(See Ref. 18)
	224TFRDX	-116.1	(Sum)	
246TFRDX				
	RDX	+14.71		4
	*	3(-40.4)		(See Ref. 18)
	246TFRDX	-106.5	(Sum)	
2244TTFRDX				
	RDX	+14.71		4
	*	2(-90.4)		(See Ref. 18)
	2244TTFRDX	-166.1	(Sum)	
2246TTFRDX				
	RDX	+14.71		4
	*	-90.4		(See Ref. 18)
	2246TTFRDX	-156.5	(Sum)	

APPENDIX Contd

		ΔH_f (kcal/mole)		Reference
MFT				
	C_6H_5F (ℓ)	-34.8		15
	C_6H_6(ℓ)	+11.7		16
	(Fluoro-)	-46.5	(Difference)	
	Tetryl(s)	+4.7		4
	MFT(s)	-41.8	(Sum)	
DFT				
	m-$C_6H_4F_2$(ℓ)	-79.6		17
	C_6H_6 (ℓ)	+11.7		16
	(Difluoro-)	-91.3	(Difference)	
	Tetryl(s)	+4.7		4
	DFT(s)	-86.6	(Sum)	

UNCLASSIFIED
Security Classification

DOCUMENT CONTROL DATA - R&D
(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1 ORIGINATING ACTIVITY *(Corporate author)* U. S. Naval Ordnance Laboratory White Oak, Silver Spring, Maryland	2a REPORT SECURITY CLASSIFICATION Confidential 2b GROUP 4

3 REPORT TITLE

Computation of Detonation Properties of Fluoroexplosives (U)

4 DESCRIPTIVE NOTES *(Type of report and inclusive dates)*

5 AUTHOR(S) *(Last name, first name, initial)*

Hurwitz, Harold

6. REPORT DATE	7a TOTAL NO OF PAGES	7b NO OF REFS
10 June 1966	41	18

8a CONTRACT OR GRANT NO	9a ORIGINATOR'S REPORT NUMBER(S) NOLTR 65-217
b PROJECT NO.	
c MIPR PG-3-19, Eglin AFB, Fla.	9b OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*
d	

10 AVAILABILITY/LIMITATION NOTICES

In addition to security requirements, which apply to this document and must be met, each transmittal outside the agencies of the U.S. Government must have prior approval of NOL.

11 SUPPLEMENTARY NOTES	12 SPONSORING MILITARY ACTIVITY
	U. S. Air Force Eglin AFB, Fla.

13. ABSTRACT

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

DD FORM 1 JAN 64 1473

UNCLASSIFIED
Security Classification

UNCLASSIFIED
Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Detonation **Fluoroexplosives** **Explosives** **RUBY**						

INSTRUCTIONS

1. ORIGINATING ACTIVITY. Enter the name and address of the contractor, subcontractor, grantee, Department of Defense activity or other organization *(corporate author)* issuing the report.

2a. REPORT SECURITY CLASSIFICATION: Enter the overall security classification of the report. Indicate whether "Restricted Data" is included. Marking is to be in accordance with appropriate security regulations.

2b. GROUP: Automatic downgrading is specified in DoD Directive 5200.10 and Armed Forces Industrial Manual. Enter the group number. Also, when applicable, show that optional markings have been used for Group 3 and Group 4 as authorized.

3. REPORT TITLE: Enter the complete report title in all capital letters. Titles in all cases should be unclassified. If a meaningful title cannot be selected without classification, show title classification in all capitals in parenthesis immediately following the title.

4. DESCRIPTIVE NOTES. If appropriate, enter the type of report, e.g., interim, progress, summary, annual, or final. Give the inclusive dates when a specific reporting period is covered.

5. AUTHOR(S). Enter the name(s) of author(s) as shown on or in the report. Enter last name, first name, middle initial. If military, show rank and branch of service. The name of the principal author is an absolute minimum requirement.

6. REPORT DATE. Enter the date of the report as day, month, year, or month, year. If more than one date appears on the report, use date of publication.

7a. TOTAL NUMBER OF PAGES: The total page count should follow normal pagination procedures, i.e., enter the number of pages containing information.

7b. NUMBER OF REFERENCES: Enter the total number of references cited in the report.

8a. CONTRACT OR GRANT NUMBER. If appropriate, enter the applicable number of the contract or grant under which the report was written.

8b, 8c, & 8d. PROJECT NUMBER: Enter the appropriate military department identification, such as project number, subproject number, system numbers, task number, etc.

9a. ORIGINATOR'S REPORT NUMBER(S). Enter the official report number by which the document will be identified and controlled by the originating activity. This number must be unique to this report.

9b. OTHER REPORT NUMBER(S). If the report has been assigned any other report numbers *(either by the originator or by the sponsor)*, also enter this number(s).

10. AVAILABILITY/LIMITATION NOTICES: Enter any limitations on further dissemination of the report, other than those imposed by security classification, using standard statements such as:

(1) "Qualified requesters may obtain copies of this report from DDC."

(2) "Foreign announcement and dissemination of this report by DDC is not authorized."

(3) "U. S. Government agencies may obtain copies of this report directly from DDC. Other qualified DDC users shall request through

_____."

(4) "U. S. military agencies may obtain copies of this report directly from DDC. Other qualified users shall request through

_____."

(5) "All distribution of this report is controlled. Qualified DDC users shall request through

_____."

If the report has been furnished to the Office of Technical Services, Department of Commerce, for sale to the public, indicate this fact and enter the price, if known.

11. SUPPLEMENTARY NOTES: Use for additional explanatory notes.

12. SPONSORING MILITARY ACTIVITY. Enter the name of the departmental project office or laboratory sponsoring *(paying for)* the research and development. Include address.

13 ABSTRACT: Enter an abstract giving a brief and factual summary of the document indicative of the report, even though it may also appear elsewhere in the body of the technical report. If additional space is required, a continuation sheet shall be attached.

It is highly desirable that the abstract of classified reports be unclassified. Each paragraph of the abstract shall end with an indication of the military security classification of the information in the paragraph, represented as *(TS), (S), (C), or (U)*

There is no limitation on the length of the abstract. However, the suggested length is from 150 to 225 words.

14 KEY WORDS. Key words are technically meaningful terms or short phrases that characterize a report and may be used as index entries for cataloging the report. Key words must be selected so that no security classification is required. Identifiers, such as equipment model designation, trade name, military project code name, geographic location, may be used as key words but will be followed by an indication of technical context. The assignment of links, roles, and weights is optional.

UNCLASSIFIED
Security Classification

Naval Ordnance Laboratory, White Oak, Md.
(NOL technical report 66-217)
COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U), by Harold Hurwitz.
10 June 1966. v.p. charts, tables.

CONFIDENTIAL

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

1. Explosives - Detonation
2. Codes - RUBY
I. Title
II. Hurwitz, Harold
III. Project

Abstract card is unclassified.

Naval Ordnance Laboratory, White Oak, Md.
(NOL technical report 66-217)
COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U), by Harold Hurwitz.
10 June 1966. v.p. charts, tables.

CONFIDENTIAL

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

1. Explosives - Detonation
2. Codes - RUBY
I. Title
II. Hurwitz, Harold
III. Project

Abstract card is unclassified.

Naval Ordnance Laboratory, White Oak, Md.
(NOL technical report 66-217)
COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U), by Harold Hurwitz.
10 June 1966. v.p. charts, tables.

CONFIDENTIAL

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

1. Explosives - Detonation
2. Codes - RUBY
I. Title
II. Hurwitz, Harold
III. Project

Abstract card is unclassified.

Naval Ordnance Laboratory, White Oak, Md.
(NOL technical report 66-217)
COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U), by Harold Hurwitz.
10 June 1966. v.p. charts, tables.

CONFIDENTIAL

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

1. Explosives - Detonation
2. Codes - RUBY
I. Title
II. Hurwitz, Harold
III. Project

Abstract card is unclassified.

Naval Ordnance Laboratory, White Oak, Md.
(NOL technical report 65-217)
COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U), by Harold Hurwitz.
10 June 1966. v.p. charts, tables.

CONFIDENTIAL

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

1. Explosives - Detonation
2. Codes - RUBY
I. Title
II. Hurwitz, Harold
III. Project

Abstract card is unclassified.

Naval Ordnance Laboratory, White Oak, Md.
(NOL technical report 65-217)
COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U), by Harold Hurwitz.
10 June 1966. v.p. charts, tables.

CONFIDENTIAL

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

1. Explosives - Detonation
2. Codes - RUBY
I. Title
II. Hurwitz, Harold
III. Project

Abstract card is unclassified.

Naval Ordnance Laboratory, White Oak, Md.
(NOL technical report 65-217)
COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U), by Harold Hurwitz.
10 June 1966. v.p. charts, tables.

CONFIDENTIAL

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

1. Explosives - Detonation
2. Codes - RUBY
I. Title
II. Hurwitz, Harold
III. Project

Abstract card is unclassified.

Naval Ordnance Laboratory, White Oak, Md.
(NOL technical report 65-217)
COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U), by Harold Hurwitz.
10 June 1966. v.p. charts, tables.

CONFIDENTIAL

The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.

1. Explosives - Detonation
2. Codes - RUBY
I. Title
II. Hurwitz, Harold
III. Project

Abstract card is unclassified.